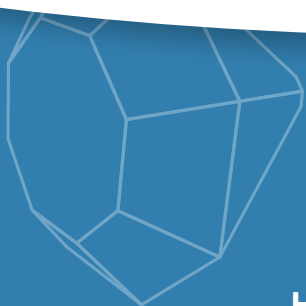


# 55<sup>th</sup> EHPRG Meeting 3-8 September 2017 POZNAŃ, POLAND

[www.ehprg2017.org](http://www.ehprg2017.org)



55<sup>th</sup> European High Pressure  
Research Group Meeting:  
High Pressure Science and Technology



**PROGRAMME**

# Programme Overview

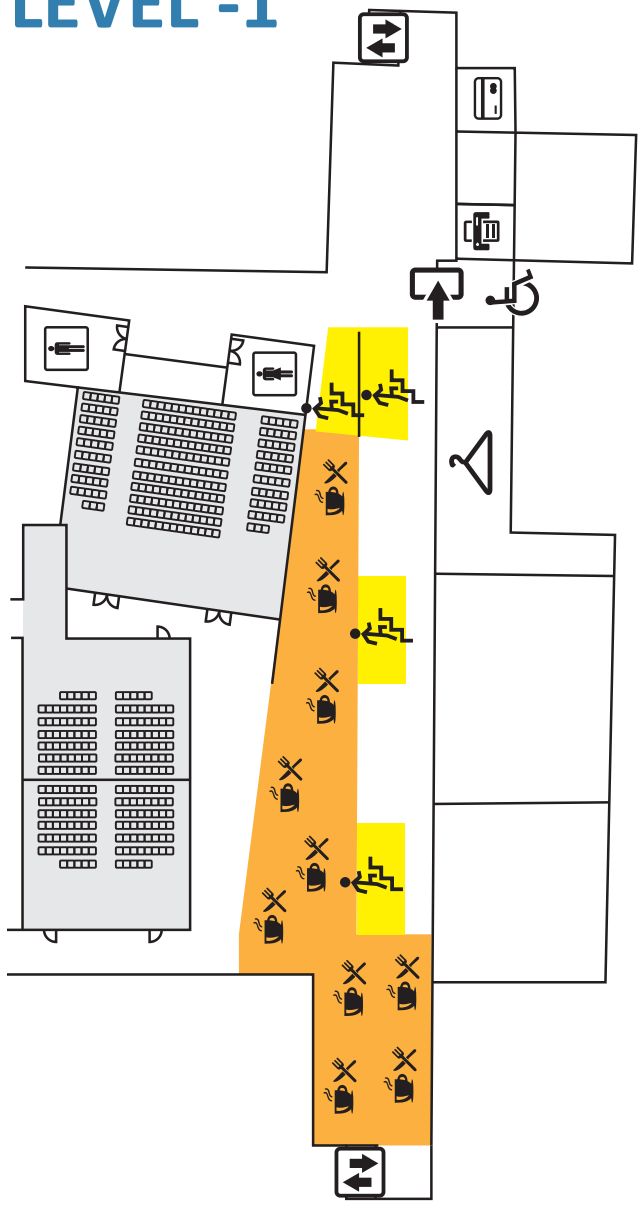
## 55th EHPRG Poznań, 3-8 September 2017

Time schedule	Sunday, 3 September 2017	Monday, 4 September 2017	Tuesday, 5 September 2017	Wednesday, 6 September 2017	Thursday, 7 September 2017	Friday, 8 September 2017	Time schedule
8.00-8.30		Registration	Registration	Registration	Special Session: Morasko Meteorite Reserve	Registration	8.00-8.30
8.30-9.00		<b>Opening Ceremony 8.45</b>	<b>PL2 - Natalia Dubrowinskaia</b> Room 2.64	<b>PL3 - Chris Michiels</b> Room 2.64	<b>Miroslaw Makohonienko</b> Start in Room 2.64		8.30-9.00
9.00-9.30		<b>PL1 - Ho-Kwang Mao</b> Room 2.64	<b>PL2 - Natalia Dubrowinskaia</b> Room 2.64	<b>PL3 - Chris Michiels</b> Room 2.64		<b>PL5 - Przemyslaw Dera</b> Room 2.64	9.00-9.30
9.30-10.00							9.30-10.00
10.00-10.30		Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break	10.00-10.30
10.30-11.00		<b>S 1 S 2 S 3</b> 2.64 2.61 3.65 2.62	<b>S 9 S 10 S 11 S 12</b> 2.62 2.61 3.65 2.64	<b>S 17 S 18 S 20</b> 3.65 2.62 2.64	<b>S 22 S 23 S 24</b> 2.62 3.65 2.64	<b>S 26 S 27 S 28</b> 2.62 3.65 2.64	10.30-11.00
11.00-11.30							11.00-11.30
11.30-12.00							11.30-12.00
12.00-12.30							12.00-12.30
12.30-13.00		Lunch Break	Lunch Break	EHPRG General Assembly Room 2.64	Lunch Break/Special Session: "Women Under Pressure gathering" Room 2.57	<b>Closing Ceremony 12.40</b>	12.30-13.00
13.00-13.30						Lunch	13.00-13.30
13.30-14.00			<b>EHPRG Group Photo</b>				13.30-14.00
14.00-14.30		<b>S 5 S 4 S 7</b> 2.64 2.61 3.65 2.62	<b>S 13 S 14 S 15 S 16</b> 3.65 2.61 2.64 2.62	Lunch Break	<b>PL4 - Elena Bolobyeva</b> Room 2.64		14.00-14.30
14.30-15.00							14.30-15.00
15.00-15.30							15.00-15.30
15.30-16.00							15.30-16.00
16.00-16.30		Coffee Break			Poster Session 2 Level 0		16.00-16.30
16.30-17.00	<b>EHPRG Committee Meeting</b> 2.57						16.30-17.00
17.00-17.30	Registration Level 0	Poster Session 1 Level 0					17.00-17.30
17.30-18.00				Excursions			17.30-18.00
18.00-18.30							18.00-18.30
18.30-19.00	Welcome Reception						18.30-19.00
19.00-19.30							19.00-19.30
19.30-20.00							19.30-20.00
20.00-20.30							20.00-20.30
20.30-21.00							20.30-21.00
21.00-21.30							21.00-21.30
21.30-22.00							21.30-22.00
22.00-22.30							22.00-22.30
22.30-23.00							22.30-23.00
					Gala Dinner Concordia Design, Zwierzyńska Street 3		

**SESSIONS:**

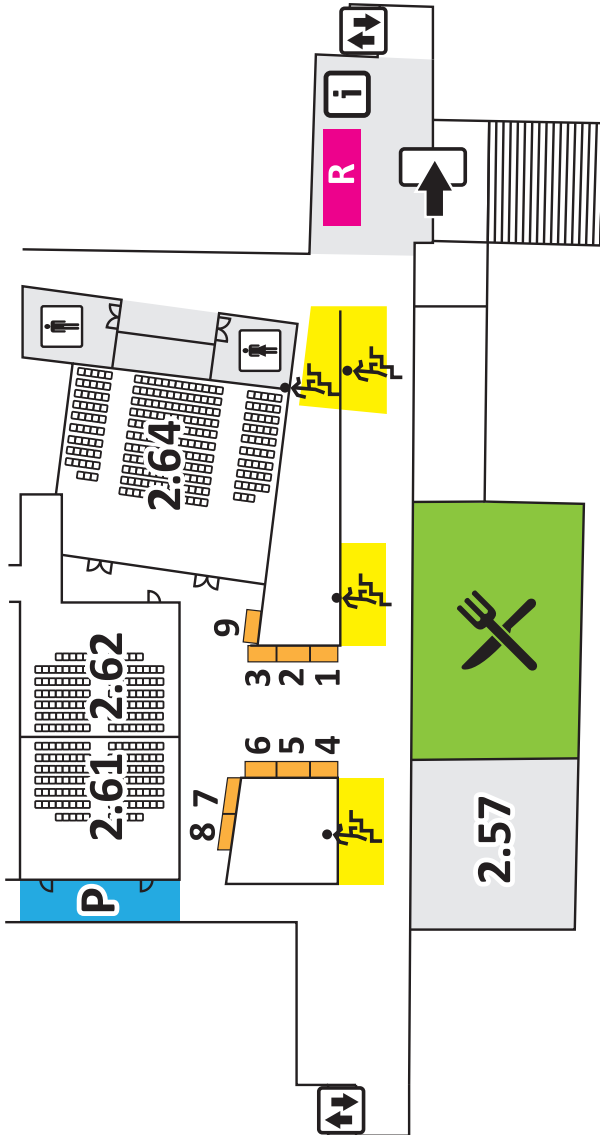
1	High-pressure chemistry
5	Materials chemistry at high pressure
11	Porous framework under pressure
15	High-pressure spectroscopy and structural studies of new materials
23	Energy materials under high pressure: experiment and theory
2	New phenomena at high pressure
4	Elements and binary alloys under pressure: structural and electronic transformations
6	Superconductivity under high pressure: experiment and theory
10	New techniques at large scale facilities
14	Pressure induced quantum criticality and novel emergent phases
26	Novel magnetic-electronic behavior at extreme P-T
18	High-pressure life and biosciences
22	Food science and technology
3	Amorphous materials and liquids under pressure
7	Critical and supercritical fluids under pressure
27	Structural phase transitions theory and experiment
8	High pressure structural analysis and (meta)data deposition
12	High pressure crystallographic studies
9	High-pressure instrumentation
13	Synchrotrons and neutron high-pressure facilities
17	Shock experiments and ultra-high pressure generation
16	Theoretical prediction of high-pressure phases
20	High-pressure studies in the Earth and planetary sciences
24	Physics and transformations in compressed matter
28	High pressure mineral physics and geochemistry
	Chemistry
	Materials
	Properties
	Biology
	Non-crystal & liquid crystals
	Method
	Theory
	Geology

# LEVEL -1



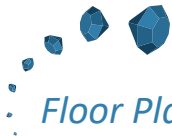
- Entrance
- Photocopy Point
- Credit Card Payment
- Coffee & Lunch Breaks
- Cloakroom
- Lifts
- Stairs
- Toilets

# LEVEL 0

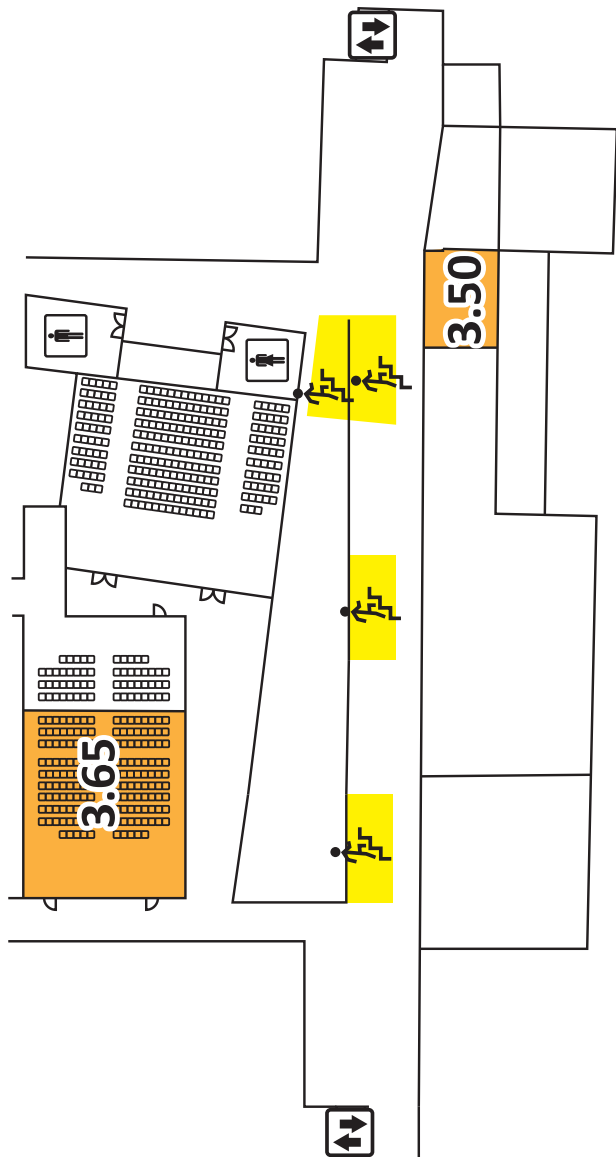


**Exhibitors:**

- |          |                        |   |               |    |                           |
|----------|------------------------|---|---------------|----|---------------------------|
| 2.61     | Lecture Room           | → | Main Entrance | 1. | Almax easyLab BvbA        |
| 2.62     | Lecture Room           | 🍴 | Canteen       | 2. | Bruker AXS GmbH           |
| 2.64     | Lecture Room           | ↕ | Lifts         | 3. | Sarl Betsa                |
| 2.57     | Committee Meeting Room | ↕ | Stairs        | 4. | Nova Swiss                |
| <b>P</b> | Poster Exhibition      | 🚻 | Toilets       | 5. | Rigaku Europe             |
| <b>R</b> | Registration Desk      |   |               | 6. | Micro Support Co., Ltd.   |
| <b>i</b> | Information            |   |               | 7. | Technodiamant Belgie BvbA |
|          |                        |   |               | 8. | WD Lab Grown Diamonds     |
|          |                        |   |               | 9. | CamCool Research Limited  |



# LEVEL 1



- 3.65 Lecture Room
- 3.50 Internet Room sponsored by Pressure BioSciences, Inc.
-  Lifts
-  Stairs
-  Toilets

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Programme Overview.....	1
Floor Plan of the Faculty of Chemistry .....	3
Conference Organizers .....	7
EHPRG Committee members 2017.....	8
EHPRG Scientific Committee .....	9
EHPRG Organizing Committee .....	10
Welcome Note by the Conference Chairman.....	11
Welcome Note by the Dean of Faculty of Chemistry .....	12
Welcome Note by the President of the Board of Adam Mickiewicz University Foundation .....	13
Welcome Note by the Mayor of Poznań.....	14
General Information.....	15
Social Programme.....	23
Excursions.....	25
Sport Activities .....	28
List of Exhibitors & Sponsors .....	29
Information for presenters .....	31
Legend to the Scientific Programme and posters.....	32
Plenary lecture ● Ho-Kwang Mao.....	33
Plenary lecture ● Natalia Dubrovinskaia .....	36
Plenary lecture ● Chris Michiels.....	38
Plenary lecture ● Elena Boldyreva .....	41
Plenary lecture ● Przemysław Dera.....	44
Open lecture ● Leonid Dubrovinsky.....	48
Special session ● Mirosław Makohonienko.....	50
Programme Overview ● Chairs & Speakers.....	53
Scientific programme ● Monday, 4 September 2017 .....	56
Scientific programme ● Tuesday, 5 September 2017 .....	63
Scientific programme ● Wednesday, 6 September 2017 .....	70
Scientific programme ● Thursday, 7 September 2017.....	73
Scientific programme ● Friday, 8 September 2017 .....	76
Poster presentations ● Monday, 4 September & Thursday, 7 September 2017.....	79
Participants list .....	92

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## Conference Organisers

---

### Conference Chairs

Prof. Andrzej Katrusiak  
Adam Mickiewicz University in Poznań  
Faculty of Chemistry  
Department of Materials Chemistry  
Umultowska Street 89b, 61-614 Poznań

Prof. Paweł Piszora  
Adam Mickiewicz University in Poznań  
Faculty of Chemistry  
Department of Materials Chemistry  
Umultowska Street 89b, 61-614 Poznań

### Conference Management

MultiBOK – Conference Organizing Bureau  
Poznan Science and Technology Park  
Adam Mickiewicz University Foundation

Rubież Street 46, 61-612 Poznań  
Phone: 61 827 97 28  
ehprg2017@ppnt.poznan.pl  
www.ehprg2017.org

**ISBN 978-83-732640-8-7**





- K. V. Kamenev, The University of Edinburgh, UK, Chairman (2018)
- N. Dubrovinskaia, University of Bayreuth, Bayreuth, Germany, Secretary (2018)
- I. Loa, CSEC, University of Edinburgh, Edinburgh, UK, Treasurer (unlimited)
- S. Klotz, Université P&M Curie, Paris, France, Treasurer Delegate (unlimited)
- R. Ahuja, Uppsala University, Uppsala, Sweden (2019)
- N. Brooks, Imperial College London, U.K. (2018)
- S. Buga, TISNCM, Troitsk, Russia (2018)
- D. Christofilos, Aristotle University of Thessaloniki, Greece (2019)
- J. Contreras-Garcia, Université P&M Curie, Paris (2018)
- A. Friedrich, Goethe-Universität Frankfurt, Germany (2017)
- G. Gabarino, ESRF, Grenoble, France (2017)
- F. Gorelli, Università di Firenze, Italy (2017)
- I. Hernandez, Universidad de Cantabria, Santander, Spain (2019)
- D. Machon, ILM - Université Lyon 1, Lyon, France (2019)
- F. Meersman, Antwerp University, Belgium (2017)
- M. Paz-Pasternak, Tel Aviv University, Israel (2017)
- M. Podsiadło, Adam Mickiewicz University, Poznań, Poland (2019)
- J. Prchal, Charles University, Prague, Czech Republic (2017)
- J. M. Recio, Universidad de Oviedo, Spain (2017)
- J. Saraiva, University of Aveiro, Portugal (2018)
- S. Scandolo, ICTP, Trieste, Italy (2018)

(Expiration dates are in parentheses)

### Ex-officio members

- F. Rodríguez, Universidad de Cantabria, Spain, President of the AIRAPT
- Cornelis Van Der Beek, École Polytechnique, Palaiseau, France, Chairman of the Condensed Matter Division of the European Physical Society

Andrzej Katrusiak (Chair) Adam Mickiewicz University, Poznań, Poland  
Rajeev Ahuja, Uppsala University, Sweden  
Simon Martin Clark, Macquarie University, Australia  
Valentina F. Degtyareva, Institute of Solid State Physics, RAS, Chernogolovka, Russia  
Karen Friese, Jülich Centre for Neutron Science, Germany  
Izabella Grzegory, UNIPRESS, PAS, Warsaw, Poland  
Giovanni Hearne, University of Johannesburg, South Africa  
Julian Haines, CNRS, Institut Charles Gerhardt, Université de Montpellier, France  
Clivia Heiny, University of Innsbruck, Austria  
Janusz Jurczak, Institute of Organic Chemistry, PAS, Poland  
Haozhe Liu, Center for High Pressure Science and Technology Advanced Research, Beijing, China  
Mohamed Mezouar, European synchrotron Research Facility, France  
Laszlo Smeller, Semmelweis University, Budapest, Hungary  
Marek Tkacz, Institute of Chemical Physics, PAS, Warsaw, Poland  
Takehiko Yagi, University of Tokyo, Japan  
Bo Zou, State Key Laboratory of Superhard Materials, Jilin University, China  
Konstantin V. Kamenev, University of Edinburgh, UK (chairman of EHPRG)  
Natalia Dubrovinskaia, University of Bayreuth, Germany  
Inge Loa, University of Edinburgh, UK  
Stefan Klotz, Universite Pierre et Marie Curie, France  
Ioannis Arvanitidis, Aristotle University, Thessaloniki, Greece  
Sergei Buga, Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Russia  
Alexandra Friedrich, Julius Maximilians University, Wuerzburg, Germany  
Julia Contreras-Garcia, Universite Pierre et Marie Curie, France  
Jesus Gonzalez, Universidad de Cantabria, Santander, Espania  
Federico A. Gorelli, Universita de Firenze, Italy  
Ulrich Häussermann, Stockholm University, Sweden  
Filip Meersman, Antwerp University, Belgium  
Moshe Paz-Pasternak, Tel Aviv University, Israel  
Jiří Prchal, Charles University, Prague, CzR  
Jose M. Recio Muñiz Universidad de Oviedo, Espania  
Alfonso San Miguel, Universite de Lyon, France  
Jorge Saraiva, University of Aveiro, Portugal  
Sandro Scandolo, ICTP, Triest, Italy  
Malcolm McMahon, University of Edinburgh, UK  
Francesca Fabbiani, University of Göttingen, Germany  
Renata Wentzcovitch, University of Minnesota, USA



Prof. Andrzej Katrusiak chairman  
Prof. Paweł Piszora vice chairman  
Dr Jolanta Darul  
Dr Anna Olejniczak  
Dr Marcin Podsiadło  
Dr Małgorzata Ratajczak-Sitarz  
Ms. Hanna Piotrowicz



## Welcome Note by the Conference Chairman

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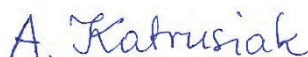


Dear Participants of the 55<sup>th</sup> EHPRG Meeting in Poznań,  
Hi Pressure Friends!

I consider it to be a distinction for our University to host this major conference of the high-pressure community. I believe that this has come as a recognition of our long tradition of high-pressure research in Poland and in Poznań. Indeed, in Poznań alone there are several groups intensively applying high-pressure in their research.

The International Advisory Board and Session Chairs did everything they could for making the program as attractive as possible, and personally I am looking forward to attend many presentations, and to meet their authors! I am very indebted to the Chairs of sessions and to Authors for contributing to the success of this Meeting. We have done everything we could to make your stay here as pleasant as possible. I am indebted to the Dean of the Chemistry Faculty for inviting the Meeting to the Collegium Chemicum building and for his constant interest and involvement in the organization matters. I believe that you will find this venue comfortable. Its surrounding offers pleasant green space for relax, sport facilities and is also conveniently connected with various attractive locations in the City. There are few cities as historical as Poznań: the cradle of Poland, the dwelling place of the first Polish dukes and kings, once the largest fortification in Europe, as well as an academic centre of a long tradition, not necessarily successful in overcoming stormy meanders of history, particularly those connected to its role as the stronghold. Presently it is a lively academic, sport, conference, transport and tourist city. I am grateful to all those actively involved in organizing this Meeting, this Faculty members, Adam Mickiewicz University and its foundation – the official Organizers. We are still around to meet your requests!

Thanks to all of you for coming!  
I wish you all success and lots of pleasure during your stay in Poznań!



Andrzej Katrusiak

Chair of 55<sup>th</sup> EHPRG Meeting

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## Welcome Note by the Dean of Faculty of Chemistry

---



Ladies and Gentlemen,

Dear Colleagues,

Welcome to Poland! Welcome to Poznań!

It is our great honor and privilege to welcome you to Faculty of Chemistry, Adam Mickiewicz University, host of 55<sup>th</sup> European High Pressure Research Group Meeting.

Poznań is an old and beautiful city, one of the largest academic and research centers in Poland. Every year thousands of students pursue their studies here. They have become part of Poznań's life and tradition. Also, Poznań is the place where Poland was born over a thousand years ago. This may also give you a special feeling of being in the very heart of Poland. For some of you it may be the first visit in Poland – so collect unforgettable memories for our country. To those of you who have seen our country years ago, it may be nice to see Poland grow and get more beautiful every day. Our new Campus Morasko, including new Collegium Chemicum, where the EHPRG meeting is held is a good example of that. At the beginning of XXI Century we must admit, that the research in such areas as chemistry, biology, pharmacy, material sciences will set standards for prosperity and a better living conditions of humankind. These sciences will have to address and resolve many problems of today's life. We do hope that the European High Pressure Research Group Meeting will take part in this challenge.

Thanks again for attending 55<sup>th</sup> European High Pressure Research Group Meeting. Thanks for visiting Faculty of Chemistry, Adam Mickiewicz University in Poznań.

Henryk Koroniak

Dean and Professor of Chemistry

Poznań, September 2017



## Welcome Note by the President of the Board of Adam Mickiewicz University Foundation

---



Dear Delegates,

I am happy to welcome you at 55<sup>th</sup> EHPRG Meeting in Poznań! Straight after choosing us as the organiser of this prestigious event, we started to look for ways to make this event special. We have put in maximum effort to ensure that you find the participation in the EHPRG Meeting as well as a productive and interesting experience.

Adam Mickiewicz University Foundation together with its key department Poznań Science and Technology Park initiated a number of activities in the field of science and economic cooperation and development of new technologies. Moreover, the Park is an experienced and reliable partner with sufficient resources and strong background in organizing conferences. Our Conference Organizing Bureau specializes in organization of conferences and seminars, meetings and conventions. For over a year we were concentrated to coordinate the EHPRG conference preparation as effective as possible.

I have no doubt that the Conference will offer all the Participants a big chance to share the knowledge with experts and industry leaders. I hope you'll also find Poznań as an attractive location for its natural, historical and cultural amenities.

Wishing you a productive and enjoyable time in hospitable Poznań!

Prof. Jacek Guliński

President of The Board of Adam Mickiewicz University Foundation

Director of Poznan Science and Technology Park



## Welcome Note by the Mayor of Poznań

---



Dear Sir or Madame,

Poznań is a city where conferences, congresses and meetings have been held for many years. More than three thousands of these events per year take place here, including many prestigious, international ones.

Thanks to Poznań's academic centers, as well as ambitious scientific projects conducted by Adam Mickiewicz University, our city is gaining the status of a leading metropolis in Poland.

The local authority's priority is therefore to undertake activities supporting universities to take initiatives, especially conferences and symposia being a platform for exchanging thoughts and experiences, in which the areas of science and business permeate.

Fifty fifth edition of the European High Pressure Research Group Meeting: High Pressure Science and Technology is an event that perfectly fits the academic and conference nature of Poznań.

I am convinced, that the potential and charm of the city with near a thousand years of history and the modern attractions, will make Poznań an ideal place to organize your meeting, which will be fruitful for all its participants.

I wish you a pleasant stay in Poznań!

Jacek Jaśkowiak

Mayor of Poznań

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## General Information

---

### Venue

Adam Mickiewicz University in Poznań  
Faculty of Chemistry  
Umultowska Street 89b, 61-614 Poznań

### Date

3-8 September 2017

### Conference Language

The lectures will be held in English.

### Registration

The Registration Desk will be open during the following times:

Sunday	16.00-19.00
Monday-Friday	8.00-10.00

Please be prepared to present your ID and, if applicable, a proof of your student status. On-site registration is also possible and credit card payment will be accepted. Registration fees are as follows:

Regular	560 EUR
Student	460 EUR
Accompanying person	460 EUR
Senior	330 EUR

### Name Badge

Participants, accompanying persons and exhibitors are kindly requested to wear their name badge during all conference events. Admittance to the scientific sessions, exhibition and social events will be refused if the required badge cannot be presented. Lost badges will be replaced at the Registration Desk upon presentation of an identity card. The name badge entitles to travel all public transport lines in Poznań. Badge is valid only with ID.



### Certificates of Participation

Certificates of Participation will be issued together with the conference package.

### WLAN and Internet Area

A wireless network will be available throughout the whole building and will be free of charge.

Login: **EHPRG**

Access code: **ehprg\_2017**

### Catering

Free lunches and soft drinks will be offered to all participants during Lunch Breaks at the catering area. Tee and coffee will be available free of charge in the morning and in the afternoon during Coffee Breaks.

### Exhibition

EHPRG 2017 will host a trade exhibition. For a listing of the exhibitors please refer to the corresponding section in this programme.

### Exhibition Opening Times

Sunday	16.00-19.00
Monday, Tuesday, Thursday	09.00-18.00
Wednesday	09.00-14.00
Friday	09.00-10.30

### Hotel Accomodation

A broad range of hotels as well as budget accomodation are available in Poznań. Please see <http://www.ehprg2017.org/hotels> for more details.



### **Venue & Travel**

#### **Conference venue**

Adam Mickiewicz University in Poznań  
Faculty of Chemistry  
Umultowska Street 89b, Poznań

#### **Sport facilities venue**

Adam Mickiewicz University in Poznań  
Department of Physical Education and Sport  
Zagajnikowa Street 9, Poznań

#### **Open lecture venue**

Auditorium of Adam Mickiewicz University,  
Wieniawskiego Street 1, Poznań

---

## Gala Dinner venue

Concordia Design,  
Zwierzyniecka Street 3, Poznań

Detailed city map is enclosed to the conference materials.

The Faculty of Chemistry owns an outdoor parking (free of charge). For planning a trip by the public transport please visit page <https://www.ztm.poznan.pl/en/#planner>. Link can be found on the conference site in the tab Venue.

We recommend to reach the conference venue by public transport.

### From Poznań-Ławica Airport to Poznań Main Railway Station („Poznań Główny”):

Bus line no. 59

Estimated time: 20 min.

Getting on: bus stop „Port Lotniczy Ławica”

Getting off: bus stop „Poznań Główny”

### From Poznań Main Railway Station to Faculty of Chemistry:

Tram lines no. 14 or 15

Estimated time: 15 min.

Getting on: tram stop „Dworzec Zachodni”

Getting off: tram stop „Os. Sobieskiego” + 10 min of walk (see map, page 23).

The Auditorium of Adam Mickiewicz University is marked on map (see page 22).

### From Mercure Hotel/Sheraton Hotel/Jowita Dormitory/Concordia Design to Faculty of Chemistry

Tram lines no. 14 or 15

Estimated time: 12 min.

Getting on: tram stop „Rondo Kaponiera”

Getting off: tram stop „Os. Sobieskiego” + 10 min of walk (see map, page 23).

## Uber

You can use Uber services in Poznań.



## General Information

---

### TAXI numbers in Poznań:

Taxi Poznań	+48 61 8 222 222
Hallo Taxi	+48 61 8 216 216
PST	+48 61 8 519 519
Radio Taxi	+48 61 8 515 515
Taxi Express	+48 601 480 480

### Currency

The currency in Poland is Polish zloty, which is approximately 0,25 euros.

### EHPRG Committee Meeting

Date: Sunday, 3 September 2017

16.00 - 18.00

Room: 2.57

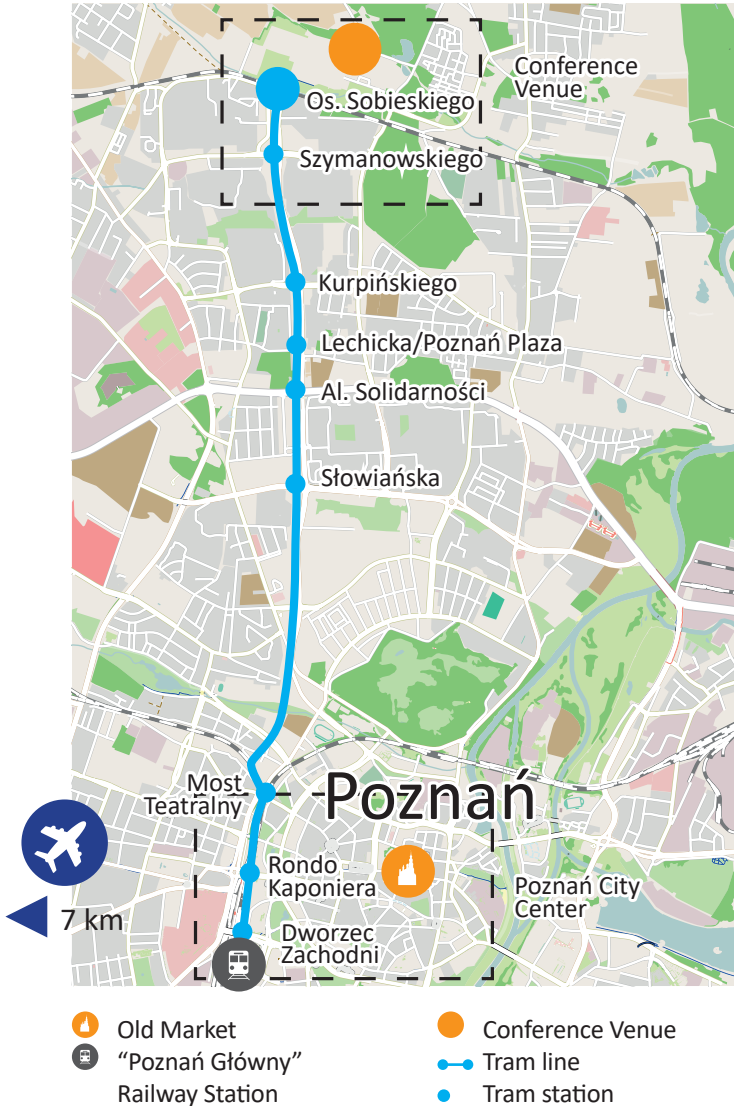
### EHPRG Group Photo

The EHPRG Community Photo will be taken on Tuesday, 5 September 2017 from 13.30 to 14.00 at the Conference Hall.

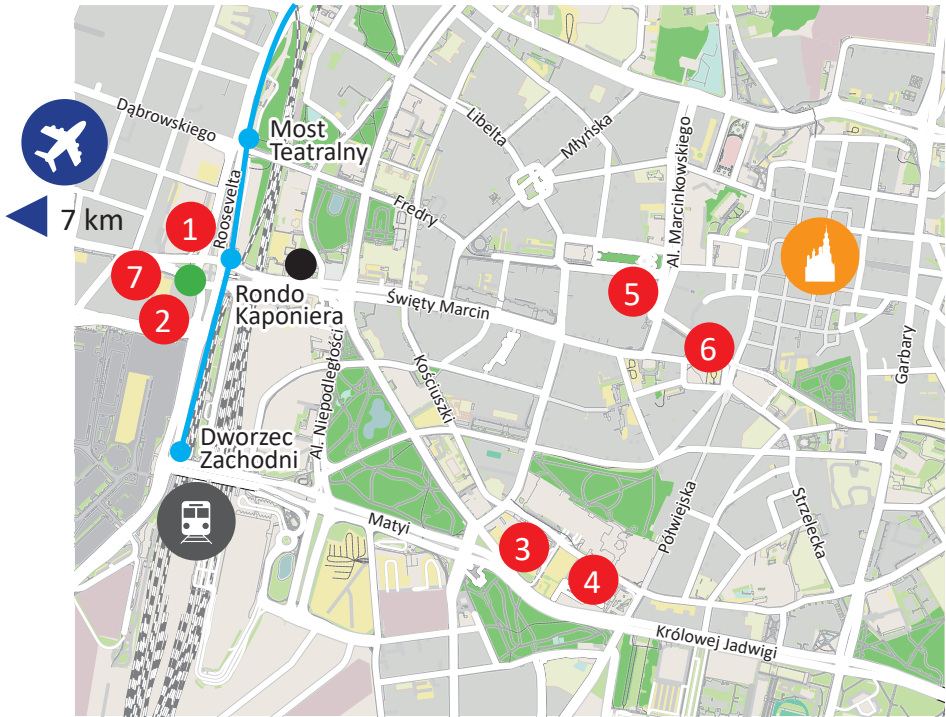
### EHPRG General Assembly

The EHPRG General Assembly will take place on Wednesday, 6 September 2017 from 12.30 to 14.00 at Room 2.64, Faculty of Chemistry, Adam Mickiewicz University in Poznań.

# Poznań City Map

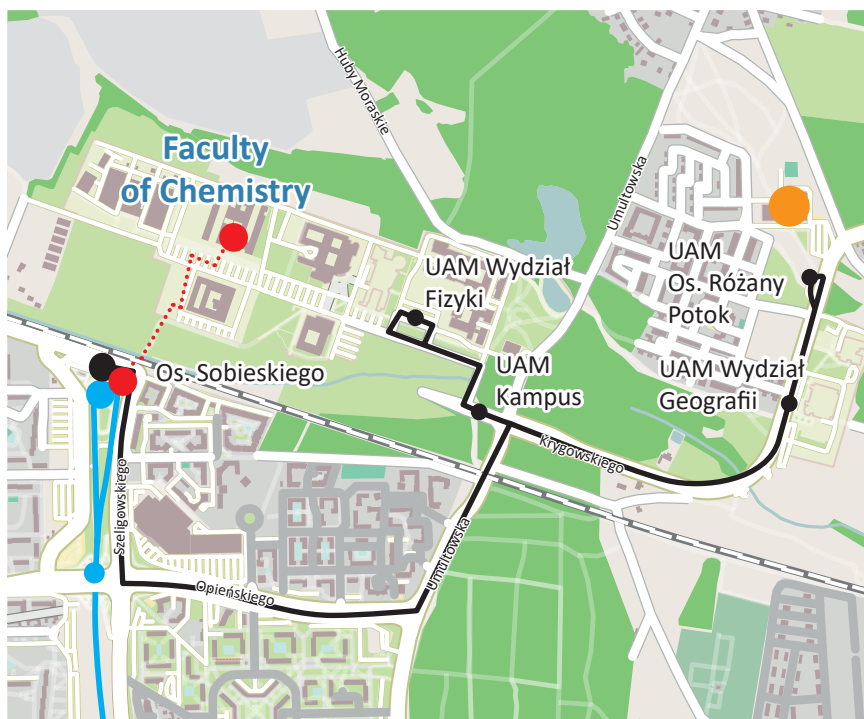








# Poznań City Center



- 1 Mercure Hotel Poznań Centrum
- 2 Sheraton Poznań Hotel
- 3 Novotel Poznań Centrum
- 4 IBB Andersia Hotel Poznań Centrum
- 5 Hotel Rzymski
- 6 Don Prestige Residence Poznań
- 7 Jowita Dormitory
- The Auditorium of Adam Mickiewicz University (Open Lecture Venue)
- "Poznań Główny" Railway Station
- Old Market Square
- Concordia Design (Gala Dinner Venue)
- Tram line
- Tram station

# Conference Venue



-  Route from the tram stop to the Conference Venue (c.a. 10 min. by foot)
-  Bus line no. 98
-  Bus station
-  Tram line
-  Tram station
-  Sport Activities venue

### **Welcome Reception**

Date: Sunday, 3 September 2017

Venue: Main Hall

Start: 18.00

The welcome evening will be graced by guitarist Matthew Kelly.

Matthew Kelly is an Irish guitarist, who has been stationed in Poznan for several years and plays eclectic music from the border of jazz and ambient, but also such genres as funk, soul, blues, salsa, swing and reggae.

If you are interested in acoustic performance of greatest hits in music entertainment feel free to enjoy the first meeting with other delegates in a relaxed atmosphere with music and light refreshments.

The Welcome Reception is included in the registration fee. On Sunday the registration will be open from 16.00 to 19.00.

### **Opening Ceremony**

The 55<sup>th</sup> EHPRG Meeting 2017 will officially be opened on Monday, 4 September 2017 at 08.45 at Room 2.64. The EHPRG Chair and Conference Chair will welcome all delegates.

### **Gala Dinner**

Date: Thursday, 7 September 2017

Venue: Concordia Design, Zwirzyniecka Street 3

Start: 19.00

The Gala Dinner will take place on Thursday, 7 September 2017 at 19.00 at Concordia Design, (Zwirzyniecka Str. 3), secession style building of the former printing house. It is located 20 minutes away from the conference venue and in the close neighborhood of Mercure Hotel and Jowita Dormitory.

This year, the gala dinner will feature an outstanding young pianist, Jacek Kortus. In February 2005 the artist was a participant in the Fryderyk Chopin Polish Piano Competition in Warsaw. In October 2005 he became a finalist, honored at the XV International Chopin Piano Competition in Warsaw.

Please note that the transport is not assured.

Required formal attire.



---

### Open Lecture

Date: Tuesday, 5 September 2017

Venue: Auditorium of Adam Mickiewicz University, Wieniawskiego Street 1

17.30-18.00      Introductory presentation: "Life in extreme conditions: Can we colonize Venus and Mars?"

Szymon Sobczak (Poznań/Poland), Michał Andrzejewski (Bern/Switzerland)

18.00-19.30      Open Lecture: "Journey to the center of the Earth 150 years after Jules Verne: Science-not fiction"

Leonid Dubrovinsky (Bayreuth/Germany), N. Dubrovinskaia

In a science fiction novel published by Jules Verne in 1864 travelers to the center of the Earth encountered "crystals...like globes of light". One hundred and fifty years later, studies of crystals compressed to enormous pressure exceeding millions of atmospheres are shining light on the inner Earth.

### Special Session

"Morasko Meteorite Reserve"

Date: Thursday, 7 September 2017

Start in Room: 2.64

8.00-10.00

### Special Session

"Women Under Pressure gathering"

Date: Thursday, 7 September 2017

Room: 2.57

12.30-14.00

### Closing Ceremony

The farewell will take place directly after the final sessions including the Closing Ceremony at the conference hall on Friday, 8 September 2017 at 12.40.

### Trip 1 - Rogalin Palace (optional), Wednesday, 6 September 2017

🕒 Duration: around 4h

The Rogalin Palace is a true jewelry of 18<sup>th</sup> century residential palace architecture. Built in the late 1700's, it belonged to a noble family of Raczyński and has been a witness to various historical events in the last 200 years. Thanks to the recent interior renovation, it now faithfully illustrates the life of various family members from late 18th century to the outbreak of WWII.



Apart from the interiors, the adjacent painting gallery of Edward Aleksander Raczyński exhibits approximately 250 works of art by acclaimed European artist. The biggest attraction, however, is painting by Jan Matejko – Joan of Arc reaching as much as 484 x 973 cm. The palace is surrounded by a French and English style gardens, the latter a home to numerous age-old oaks, including the country-famous Lech, Czech and Rus.



You are going to see richly furnished rooms with work-of-art chandeliers, cutlery, paintings and many other examples of applied arts. The library room, with its wooden hand-carved bookcases covering all 4 walls a few meters all the way up to the ceiling is considered the greatest highlight of the palace.



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**Trip 2 - Poznań (optional), Wednesday, 6 September 2017**

🕒 Duration: around 3h



Poznań - the 5<sup>th</sup> biggest city in Poland and the capital of the Greater Poland province has a history spanning across more than 1,000 years. On this trip you are going to dive back to the roots of the city located on Ostrów Tumski (the Cathedral Island) and explore 10<sup>th</sup> century, relicts hidden beneath the cathedral floor. You will witness the very beginnings of the Polish state and Christianity on that territory.

Next, you are going to the colourful Market Square with the 16<sup>th</sup> century, Renaissance Town Hall towering over the city. It is here, every day at noon that the famous goats of Poznań appear in front of crowds gathering to watch the show. Other spots on the itinerary include a true jewelry of Roman Baroque: the former Jesuits church of St. Stanislaw the Bishop, adjacent palaces and the Royal Castle topping the Przemyslaw Hill. The tour will be finished on a sweet note – a tasting of St. Martin Croissant, a local specialty revered by tourists.



## Trip 3 - Morasko Reserve (optional), Thursday, 7 September 2017

🕒 Duration: around 2h

Morasko Reserve was established around 6 impact craters created by meteors about 5,000 years ago. First meteor weighing 77 kg was found here in 1914 by German soldiers digging trenches. Subsequent excavations unveiled much bigger pieces – 164 and 261 kg, the last being the biggest meteor piece discovered in Poland.

The impact resulted in sizable craters, the biggest reaching around 90 meters in diameter and 11 meters of depth. On this trip you are going to see the impact craters and learn about the processes involved in meteor impacts.



## Sport Activities

Venue:

Adam Mickiewicz University in Poznań  
 Department of Physical Education and Sport  
 Zagajnikowa Street 9, Poznań

Participation in the activities is possible only after the registration at the Registration Desk (one day in advance) with valid conference ID. All facilities are included in the fee.

Sport activity	Number of people	Trainer	Opening hours	Comments
<b>Indoor swimming</b>	max 60 people	Yes (lifeguards)	6.00 – 22.00	
<b>Tennis</b>	2-8 people	Yes	6.00 – 22.00	Personal trainer: extra charge
<b>Volleyball</b>	8-36 people	Yes	10.00 – 12.00 16.00 – 18.00	
<b>Basketball</b>	8-36 people	Yes	10.00 – 12.00 16.00 – 18.00	
<b>Gym</b>	36 people	Yes	6.00 – 22.00	Personal trainer: extra charge
<b>Fencing</b>	2-10 people	Yes	6.00 – 22.00	Personal trainer: extra charge
<b>Table tennis</b>	2-8 people	Yes	6.00 – 22.00	
<b>Sauna</b>	max 10 people	Yes	6.00 – 22.00	



## List of Exhibitors & Sponsors

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### Exhibitors

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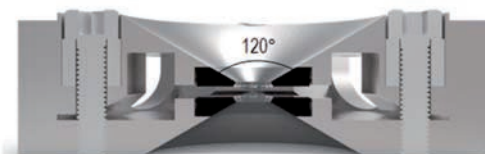




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## Information for presenters

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### Submitting your Presentation/Technical Information

Please note: Each presentation must be delivered to the lecture room at least 30 minutes before the beginning of the session. Please use an USB flash drive, CD or DVD disc which must not be protected with software.

Please prepare your presentation as PDF, MS Office Power-Point 2010/2007 for Windows or key for Macintosh DVD in 16:9 aspect ratio.

A presentation notebook with a PDF reader and MS Office Power-Point 2010/2007 will be provided. The use of personal notebooks is possible upon agreement. However, it may interrupt the flow of the programme in the lecture hall. Please provide an adapter for VGA if necessary.

A notebook and laser pointer are available at the speaker podium in the lecture rooms. A technical supervisor can help you.

Please note: Certain encodings for video and audio files could lead to problems.

### Speaking Time

Speaking time is specified in the program. Please prepare your presentation for the allotted amount of time. Session chairs are asked to interrupt you, in case that you should exceed your time limit.





## Legend to the scientific programme and posters

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Name	<u>Plenary speaker</u>
Name	<u>Invited lecturer</u>
Name	<u>Invited oral</u>
Name	<u>Presenting author</u>

<b>PL 1</b>	Plenary lecture
<b>S 1</b>	Session number
<b>IL 1.1</b>	Invited lecture
<b>IO 1.1</b>	Invited oral
<b>O 1.1</b>	Oral
<b>P</b>	Poster

### Posters

Posters are to be displayed for the entire conference in the Poster Exhibition. Authors are kindly requested to set up their poster on the corresponding board with the supplied material on Monday, 4 September before 10.00. Poster boards have the same number as the titles in the Conference Programme.

The poster session for **odd** numbers, e.g. P1, P3, P5 etc. will be held on Monday, 4 September from 16.30 to 18.30.

The poster session for **even** numbers, e.g. P2, P4, P6 etc. will be held on Thursday, 7 September from 15.00 to 17.00.

Poster presenters are kindly requested to be present during their poster sessions. Poster boards are made from cork and their size is 980 mm x 1220 mm. The posters should not be laminated. Mounting materials will be provided on-site.

### Best Poster Award

The Best Poster Award is sponsored by 55<sup>th</sup> EHPRG Meeting Organizing Committee.

The Award presentation ceremony will be held during the Closing Ceremony. All Authors who would like to participate in the competition can get a sticker at the Registration Desk to mark their posters.



*HPSTAR, Center for High Pressure Science and Technology  
Advanced Research, Shanghai, P.R. China*

**Monday, 4 September 2017, 9.00, Room 2.64**

### **Biographical sketch**

Dr. Ho-Kwang Mao is the Director of Center for High Pressure Science and Technology Advanced Research in China, and a senior staff scientist at the Geophysical Laboratory, Carnegie Institute for Science. He received Ph.D. degree in 1968 from the University of Rochester, and worked at the Geophysical Laboratory on high-pressure research ever since. He has led numerous breakthroughs in experimental high-pressure science. In the 1970-80's, he advanced the static high-pressure capabilities beyond 300 GPa which was an order of magnitude higher than the previous record, thus greatly expanding the field. Subsequently, he and his group pioneered the integration of pressure with high-temperature and cryogenic conditions and optical, electromagnetic, and synchrotron x-ray probes that enable a full range of in-situ, high P-T, condensed-matter investigations. The results have made major impacts on fundamental physics, as well as applications in geophysics and astrophysics.

Ho-Kwang Mao is a Member of the National Academy of Sciences (USA) and Academia Sinica (Taiwan), a Foreign Member of Chinese Academy of Sciences (China) and Royal Society of London (UK), and Fellow of the American Physical Society, American Geophysical Union, Geochemical Society, and European Association for Geochemistry. Among his prizes and distinctions are the Balzan Prize (Balzan Foundation), Inge Lehmann Medal (American Geophysical Union), Gregori Aminoff Prize (Royal Swedish Academy of Sciences), Roebling Medal (Mineralogical Society of America), Arthur L. Day Prize (National Academy of Sciences, USA) and P. W. Bridgman Gold Medal (AIRAPT).



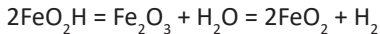
## Superoxidation, hydrogen generation, and new paradigm of the Deep Earth

Ho-Kwang (David) Mao<sup>1,2</sup> and Qingyang Hu<sup>1</sup>

<sup>1</sup> Center for High-Pressure Science and Technology Advanced Research, Shanghai, P.R. China

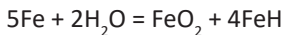
<sup>2</sup> Geophysical Laboratory, Carnegie Institution for Science, Washington, U.S.A.

Using first-principles calculations and direct experiments at 76 GPa and 1800 K, we discovered a highly stable, pyrite-structured, iron peroxide ( $\text{FeO}_2$ ) with  $Pa3$  symmetry that holds an unprecedentedly large amount of oxygen. Further study shows that the new pyrite-structured iron peroxide may be synthesized from the bog iron ore,  $\text{FeO}_2\text{H}$ , under the deep lower mantle conditions and release  $\text{H}_2$  [1]. The same reaction is also observed from the reaction of  $\text{Fe}_2\text{O}_3$  and  $\text{H}_2\text{O}$ , i.e.,



In the presence of hydrogen, the pyrite-structured iron peroxide may contain residual hydrogen,  $x$ , as  $\text{FeO}_2\text{H}_x$ , where  $x < 1$ . Using a combination of theoretical simulations and high pressure-temperature experiments, we calibrated the  $x$  dependence of molar volume of the peroxide. The high-pressure chemistry weakens the OH bonds of the peroxide structure, and the hydrogen atom is mobile in this phase. Increasing temperature and heating time helps release hydrogen and lower  $x$ , suggesting that dehydrogenation could be approaching completion at the high-temperature conditions of the lower mantle over extended geological time [2].

Although the supply of  $\text{FeO}_2\text{H}$  or  $\text{Fe}_2\text{O}_3$  is limited, we demonstrated that the peroxide can also be synthesized from the reaction of the Fe in the core and  $\text{H}_2\text{O}$ , i.e.,





When the continuous supply of water from dehydration of the down-going slab meets the inexhaustible iron at the core-mantle boundary, they will form a reaction zone with the complete sequence from iron peroxide,  $\text{Fe}_2\text{O}_3$ ,  $\text{Fe}_3\text{O}_4$ ,  $\text{FeO}$ , to metallic iron together with iron hydride. Hydrogen in the reaction zone will escape upon further heating and rise to the crust, sustaining the water cycle. Our observations indicate a fundamental change in the mode of hydrogen release from dehydration in the upper mantle to dehydrogenation in the deep lower mantle, thus differentiating the deep hydrogen and hydrous cycles. The reaction may cause accumulation of the heavy superoxidized iron oxide patches at the core mantle boundary, upward migration of the hydrogen, and separation of the oxygen and hydrogen cycles.

Acknowledgements: This work was supported by NSF Grants EAR-1345112 and EAR-1447438, and partially by the National Natural Science Foundation of China Grant U1530402.

### References

- [1] Q. Hu et al., *Nature*, 2016, **534**, 241.
- [2] Q. Hu et al., *Proc. Natl. Acad. Sci. USA* 2017, **114**, 149.



*Universität Bayreuth, Laboratory of Crystallography, Bayreuth,  
Germany*

**Tuesday, 5 September 2017, 9.00, Room 2.64**

### **Biographical sketch**

Natalia Dubrovinskaia graduated from the Department of Crystallography and Crystal Chemistry of the Faculty of Geology at Moscow State University in 1983, received her Ph.D. in crystallography and crystal physics from the same University in 1989 (supervisor: Prof. Vadim S. Urusov). Later she passed habilitation and obtained the *venia legendi* at the University of Bayreuth and the University of Heidelberg in Germany. She is currently Professor in Material Physics and Technology at Extreme Conditions at the Laboratory of Crystallography of the University of Bayreuth. Her research interests cover high pressure synthesis of novel inorganic materials including nanocrystalline materials with advanced mechanical properties, development of new scientific instruments for high and ultra-high pressure generation, as well as application of synchrotron radiation in materials science and solid state physics. Natalia Dubrovinskaia was awarded the Gregori Aminoff Prize in Crystallography 2017 of the Royal Swedish Academy of Sciences “for having developed new methodology for in situ-experimental determination of crystal structures subjected to extreme conditions of high temperature and pressure”.



### Structural studies taken to the extreme

N. Dubrovinskaia<sup>1</sup> and L. Dubrovinsky<sup>2</sup>

<sup>1</sup>Material Physics and Technology at Extreme Conditions, Laboratory of Crystallography, University of Bayreuth, D-95440 Bayreuth, Germany

<sup>2</sup>Bayerisches Geoinstitut, University of Bayreuth, D-95440 Bayreuth, Germany

Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. The most reliable information about crystal structures and their response to changes in pressure and temperature is obtained from single-crystal diffraction experiments. Advances in diamond anvil cell (DAC) techniques and double-stage DACs, as well as in modern X-ray facilities have increased the accessible pressure range for structural research up to multimegabar range. We have developed a methodology to perform single-crystal X-ray diffraction experiments in double-side laser-heated DACs. Our results demonstrated that the solution of crystal structures, their refinement, and accurate determination of thermal equations of state of elemental materials, oxides, carbides, borides, carbonates, and silicates from single-crystal diffraction data are possible above 200 GPa at temperatures of thousands of degrees. These resulted in findings of novel compounds with unusual compositions, crystal chemistry, and physical properties.



*Laboratory of Food Microbiology  
at the Faculty of Bioscience Engineering  
of the University of Leuven, Belgium*

**Wednesday, 6 September 2017, 9.00, Room 2.64**

### **Biographical sketch**

Chris Michiels is professor and head of the Laboratory of Food Microbiology at the Faculty of Bioscience Engineering of the University of Leuven (KU Leuven), Belgium. His research addresses mechanistic and quantitative aspects of the inactivation, survival and growth of foodborne bacteria throughout the food production chain, and aims to support the development of novel or improved technologies for controlling food safety and quality. The primary focus is on the mechanisms of adaptation and resistance development of foodborne bacteria towards different types of stress applied in food processing and preservation, such as heat, high pressure, cold, acid and preservatives. The research approach combines basic microbiological methods with a range of molecular, genetic and omic techniques to investigate bacterial adaptation at the molecular, cellular, population and ecosystem level. Chris Michiels has (co-)authored about 200 papers in peer-reviewed journals, and he has edited a book on high pressure microbiology. He is also editor of the International Journal of Food Microbiology.



### **Bacterial inactivation by high pressure treatment: recent insights and applications in food preservation**

C.W. Michiels<sup>1</sup>, A. Aertsen<sup>1</sup> and E. Gayan<sup>1</sup>

<sup>1</sup>Laboratory of Food Microbiology and Leuven Food Science and Nutrition Research Centre (LFOiRCe),  
Dept. of Microbial & Molecular Systems, KU Leuven, Heverlee, Belgium

In two decades, high hydrostatic pressure (HP) treatment has become established as a novel food preservation process, and several HP processed foods are currently commercially available. Similar to conventional thermal processing (pasteurization or sterilization), HP processing extends the shelf-life and increases the safety of foods by killing microorganisms that can cause spoilage or foodborne disease. Since microbial inactivation by pressure can take place at ambient or even at reduced temperature, HP processing is particularly of interest for foods that incur an unacceptable quality loss upon heating. The most successful applications are those where HP processing offers a much superior product quality than a heat treatment that is equivalent in terms of microbial reduction [1].

The inactivation of foodborne bacteria by HP has been amply documented. Generally, nonsporulated bacteria can be efficiently inactivated in a few minutes at 300-600 MPa at ambient temperature, while bacterial spores can resist up to 1000 MPa or more. However, some nonsporulated bacteria can stably acquire an extreme level of HP resistance, similar to that of spores [2]. This is remarkable because such high pressures are predicted to irreversibly denature most of the cellular enzymes in the aqueous cytosolic compartment of nonsporulated cells. The genetic analysis of extremely HP resistant mutants of *Escherichia coli* has recently revealed different mutations that can cause resistance, but how these mutations allow cells to prevent or revert damage to cellular enzymes and structures is still poorly understood [3,4].



HP resistance can not only evolve under selection pressure in the laboratory, some bacterial strains with very high HP resistance have also been isolated from their natural environment, and these are a concern for HP processed foods. Inactivation of such HP resistant bacteria requires the combination of HP treatment with another antimicrobial process or with an antimicrobial compound. Some of these combinations enhance bacterial inactivation in a synergistic manner, opening interesting perspectives for mild food preservation. Of particular interest are combinations of HP with natural antimicrobial compounds, because these allow at the same time to replace artificial food preservatives with natural alternatives [5]. An illustration of the efficacy of such a combination is shown in Figure 1. While very efficient to inactivate nonsporulated bacteria, combinations of HP and antimicrobials cannot inactivate spores. Efficient spore inactivation is only possible when HP is combined with heat.

#### References

- [1] H.-W. Huang et al., *Food Control*, 2017, **72**, 1.
- [2] K. Hauben et al., *Appl. Environ. Microbiol.*, 1997, **63**, 945.
- [3] D. Vanlint et al., *Int. J. Food Microbiol.*, 2013, **163**, 28.
- [4] Gayan et al., *Sci. Rep.*, 2017, **7**, 8600.
- [5] Feyaerts et al., *Innov. Food Sci. Em. Technol.*, 2015, **27**, 26.



*Institute of Solid State Chemistry and Mechanochemistry,  
Siberian Branch of Russian Academy of Sciences,  
Novosibirsk, Russia*

**Thursday, 7 September 2017, 14.00, Room 2.64**

### **Biographical sketch**

Chief Researcher at the Institute of Solid State Chemistry and Mechanochemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk and Head of the Chair of Solid State Chemistry of Novosibirsk State University.

Prof. Boldyreva is known for her profound studies on the reactivity of solids, high-pressure and low-temperature crystallography, polymorphism, crystallization, phase transitions, dissolution of molecular solids, problems related to mechanochemistry, drug-excipient interactions, metastable and amorphous states of molecular solids, drug formulations, photo- and thermomechanical effects, and feed-back phenomena. While the research is fundamental, it finds considerable applications in biology, pharmaceutical sciences, materials science, and related industries.

Prof. Boldyreva was one of the pioneers in the discovery and study of photomechanical effects in molecular crystals in the 1980s-1990s, and has continued this research in recent years. She has contributed to the quantitative description of various types of photomechanical effects in relation to reaction kinetics and mechanism, as well as to combining photocystallography and photospectroscopy with high-pressure research.

Prof. Boldyreva is a pioneer of high-pressure diffraction studies of organic and coordination compounds. She systematically uses high pressure as a tool to study and modify the intermolecular interactions and intramolecular conformations in crystals, to trigger polymorphic transformations, to obtain new crystalline forms, and to understand the mechanisms of dissolution, crystallization, solid-state transformations and chemical reactions. Through this work, particular attention is paid to the kinetics and control of the transformations. Prof. Boldyreva's group is the only group in Russia and one of the leading groups in the world in this field.

Prof. Boldyreva has contributed to the research of the "feed-back" phenomenon, and the related concept of the reaction cavity, by both experimental techniques and computational modeling.

Prof. Boldyreva is widely known for her profound original research of polymorphism in organic compounds. She has made significant contributions to understanding the thermodynamics and kinetics of their formation, and structure-properties relations across polymorphic series.

In addition, Prof. Boldyreva has made major original contributions in the field of organic mechanochemistry, and is actively involved in organizing international conferences in this field.

Prof. Boldyreva is also active in the study and design of new solid drug forms and formulations with improved properties. She is one of the leaders in the study of drugs and drug formulations as materials.

Prof. Boldyreva is the author and co-author of over 300 papers in peer-reviewed journals and over 30 chapters in monographs.

Prof. Boldyreva is a member of many research societies and committees, including the International Advisory Committee on the Reactivity of Solids, the European Crystallographic Association, the International Mechanochemical Association, the American Nanosociety, the COMPRES society (USA), the American Chemical Society, Sigma Xi research society, the National Committee of Russian Crystallographers, the International Committee on the Chemistry of the Organic Solid State, the International Association of Physical Chemists, the European Society of Physical Chemistry, Eurostar-Science, the German Crystallographic Society, the International Centre for Diffraction Data (2002 - present time), and the International Union of Crystallographers (IUCr). She is a member of the IUCr Commissions on High Pressure and on Teaching, and of a Special Interest Group “Intermolecular interactions and crystal chemistry”. From 2008 until 2014 she was an elected member of the Executive Committee of the IUCr.

She was a Member of the Chemistry Expert Committee of the Russian Foundation of Basic Research and acts as an expert for many foundations in Russia and abroad. She was a member of the Selection Committees for the Ewald, Perutz, and Bertaut Prizes. Prof. Boldyreva is a Member of the Advisory Council on Science of the Russian Ministry of Science and Education, and was a Member of the Advisory Council on Science and Education of the President of the Russian Federation (2012-2014).



### Coordination and organic compounds at high pressures. Retrospect and Challenges

Elena Boldyreva<sup>1</sup>

<sup>1</sup>Institute of Solid State Chemistry and Mechanochemistry SB RAS

Crystals of organic and coordination compounds were actively studied by spectroscopic techniques already in the middle of the 20 century. The effect of high pressure on the reaction kinetics was used as a key to understanding of the mechanisms of chemical reactions in solution. Since the late 1990s crystalline coordination and organic compounds are being actively studied at high pressures also by diffraction techniques. The pressures not exceeding 10 GPa are sufficient, to induce many interesting processes in these systems, including, among other, anisotropic strain, changes in molecular conformations, distortion or switching over of hydrogen bonds, proton migration, charge transfer, structural polymorphic transformations, recrystallization, solvation (more generally - formation of host-guest compounds), or, contrary, pressure-induced dehydration of crystal hydrates.

The phases formed under given temperature-pressure conditions are not necessarily the thermodynamically stable ones. Quite often the phases formed are metastable, but can be preserved during indefinitely long time. Moreover, quite often the thermodynamically stable phases cannot be formed, unless a special experimental protocol is used and a recrystallization from a fluid phase is possible. The phenomenon is termed “kinetic control” and is related to the large difference in the rates of nucleation and nuclei growth of different phases, not directly proportional to their relative stabilities. The protocol of compression and decompression, the choice of pressure-transmitting fluid or/and of the starting polymorph, the sample size, temperature, irradiation by light, the presence of other phases in the same cell, and other factors can be critically important for the formation of selected phases, their recrystallization or solid-state transformations on hydrostatic compression. High-pressure research can also elucidate the mechanisms of photo- / thermo- transformations in solids and feed-back phenomena.



*Hawaii Institute of Geophysics and Planetology,  
School of Ocean and Earth Science and Technology  
University of Hawaii at Manoa, Honolulu, U.S.A.*

**Friday, 8 September 2017, 9.00, Room 2.64**

### **Biographical sketch**

Przemysław (Przemek) Dera is a Professor of Mineral Physics and Extreme Materials Science at the Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa in Honolulu. He obtained his Ph.D. in physical chemistry in 2000 from Adam Mickiewicz University in Poznań, Poland, under tutelage of Prof. Andrzej Katrusiak. Prior to moving to Hawaii, he worked as research scientist at Carnegie Institution of Washington's Geophysical Laboratory (2000-2007) and University of Chicago's Center for Advanced Radiation Sources (2007-2013). Przemek has been closely involved in the activities of high-pressure research community both within USA, as well as internationally. He chaired the International Union of Crystallography Commission on High Pressure (2008-2014) and served as member and vice-chair the Executive Committee of COMPRES, the Consortium for Materials Properties Research in Earth Sciences (2010-2013). His main scientific interests include study of pressure-induced displacive phase transitions and spin crossover phenomena in materials, with particular emphasis on minerals relevant to planetary interiors. Przemek is an Elected Fellow of the Mineralogical Society of America (2013) and was selected as Distinguished Lecturer for COMPRES in 2015. He has authored and co-authored 99 papers in scientific journals, 4 book chapters, and co-edited 4 books and journal special volumes.



### Hypervalent penta-coordinated silicon and metastable phase transitions in silicates

Przemysław Dera<sup>1</sup>

<sup>1</sup>Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology  
University of Hawaii at Manoa, Honolulu, U.S.A.

Earth is a rocky planet, dominated by silicate minerals, which undergo chemical and physical transformations as a function of depth, and thus control properties and dynamics of the planet interior. Global geologic phenomena and processes including deep-focus earthquakes and plate tectonics are often affected by these transformations. Silicon strongly prefers four-coordinated crystallographic sites due to the  $sp^3$  electron hybridization. As a consequence, in silicate minerals characteristic of shallow Earth interior, including the crust and the upper mantle, silicon resides predominantly in tetrahedral sites coordinated by four oxygen atoms ( ${}^{\text{IV}}\text{Si}$ ). This low coordination number and mesodesmic bonds, found e.g. in quartz, pyroxene or olivine, result in significant structural flexibility for forming extended silicate chain, sheet, and framework polyhedral motifs, and accounts for majority of the structural diversity observed in terrestrial rocks of shallow origin. However, silicon is also capable of forming hypervalent, 5- and 6- coordinated states ( ${}^{\text{V}}\text{Si}$  and  ${}^{\text{VI}}\text{Si}$ ). These hypervalent states are favored at higher pressure and with increased ligand electronegativity. As a result, in the Earth interior, at greater depths and higher pressures, silicon strongly prefers sites with six nearest neighbor ligands arranged in octahedral geometry, leading to more compact, higher density phases such as  $\text{SiO}_2$  stishovite,  $(\text{Mg}, \text{Fe})\text{SiO}_3$  bridgmanite or  $\text{MgSiO}_3$  akimotoite. Densification of silicates, involving a coordination number increase from four ( ${}^{\text{IV}}\text{Si}$ ) to six ( ${}^{\text{VI}}\text{Si}$ ) accounts for much of the stratification of the Earth mantle, and is responsible for some of the major seismic discontinuities within our planet.

There has been great interest in understanding the occurrence and properties of the least common, penta-coordinated Si phases ( ${}^{\text{V}}\text{Si}$ ) both in geophysics, as well as in solid state chemistry. Stereochemical analysis of crystal structures reported to contain  $[\text{SiL}_5]$  groups in crystals with hexagonal close-packed arrays of ligands indicates that there is an almost continuous change from an  $[\text{SiL}_4]$  tetrahedron to an  $[\text{SiL}_5]$  trigonal bipyramid, and that the penta-coordinated state indeed plays a critical role as intermediate in condensation and decondensation reactions of silicates in aqueous solutions and in melts [3]. Amorphous solids, melts and liquids can sustain exotic coordination environments such as  $\text{SiO}_5$  more easily due to the lack of symmetry and long-range order. Indeed, several studies of glass and melts clearly indicate existence of penta-coordinated silicon at elevated pressures, which can sometimes persist in quenched samples. It is also believed that penta-coordinated silicon plays an important role in dissolution of silica and change of deformation mechanism [4]. At ambient conditions, crystalline silicate minerals with  ${}^{\text{V}}\text{Si}$  are rare, but have been reported previously in the literature based on both experiments and calculations. For example, a quenchable phase

with five-coordinated Si was observed in  $\text{CaSi}_2\text{O}_5$  silicate, which can be synthesized at 1500 °C and 10 GPa [5] and could be metastably quenched.

Many high pressure phases that form through displacive phase transitions are non-quenchable, and can be characterized only at elevated pressure and temperature conditions, at which they are more stable than the ambient polymorphs. Metastable paths of multi-stage displacive polymorphic transition sequences have sometimes been seen to replace direct, abrupt, reconstructive transformations to high-density thermodynamically stable structural arrangements, when temperature is sufficiently low. Such conditions are characteristic of subduction zone environments, in which the mantle convection allows low pressure minerals to be transported to significant depths while remaining at temperatures much lower than the mantle geotherm.

In this context, it seemed possible that metastable high-pressure phases of common silicate minerals involving exotic hypervalent Si could have been overlooked in earlier experiments limited either by pressure range of the available experimental techniques, or by their sensitivity to detect subtle symmetry distortions. In a quest to find such previously unknown high-pressure silicate polymorphs characterized by hypervalent  $^{\vee}\text{Si}$  and understand the geophysical consequences of their existence, we used a combination of high-pressure synchrotron X-ray diffraction and density functional theory calculations to systematically explore two large families of chain silicate minerals, pyroxenes and amphiboles. This presentation will review systematic phase transition trends and new structural varieties that have been discovered. We investigated the structural aspects of the new transformations and their effects on lattice preferred orientation and transformation fabrics of the high-pressure metamorphic rocks. The results suggest that the presence of  $^{\vee}\text{Si}$  has consequences for chemical reactivity, elastic anisotropy, elastic and plastic deformation, density of the subducted slab and affects buoyancy relative to the surrounding mantle.

Acknowledgements: The project was supported by the National Science Foundation Division of Earth Sciences Geophysics grant 1344942. Development of the ATREX software, used for experimental data analysis was supported by NSF EAR Geoinformatics grant 1440005. Portions of the X-ray diffraction work were conducted using X-ray Atlas instrument at the University of Hawaii, funded by NSF EAR Instrumentation and Facilities grant 1541516. Portions of this work were performed at GeoSoilEnviroCARS (Sector 13), Advanced Photon Source (APS), Argonne National Laboratory. GeoSoilEnviroCARS is supported by the National Science Foundation—Earth Sciences (EAR-1128799) and Department of Energy—Geosciences (DE-FG02-94ER14466). Use of the Advanced Photon Source was supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

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Bayerisches Geoinstitut University of Bayreuth,  
Bayreuth, Germany

**Tuesday, 5 September 2017, 18.00,  
The Auditorium of Adam Mickiewicz University  
Wieniawskiego Street 1, Poznań**

### Biographical sketch

Leonid Dubrovinsky graduated from the Department of Crystallography and Crystal Chemistry of the Faculty of Geology at Moscow State University in 1983, received his Ph.D. from the same University in 1986 (supervisor: Prof. Vadim S. Urusov). He obtained the *venia legendi* at Uppsala University in Sweden and the University of Bayreuth in Germany. He is currently Academic Director at the Bavarian Research Institute of Experimental Geochemistry and Geophysics (Bayerisches Geoinstitut) in Bayreuth. His research interests cover high pressure studies of geophysically important materials, high pressure solid state physics and chemistry, development of new scientific instruments for structural studies at high pressures and temperatures. Leonid Dubrovinsky was awarded the Gregori Aminoff Prize in Crystallography 2017 of the Royal Swedish Academy of Sciences “for having developed new methodology for *in situ*-experimental determination of crystal structures subjected to extreme conditions of high temperature and pressure”.

## Journey to the center of the Earth 150 years after Jules Verne: Science - not fiction

L. Dubrovinsky<sup>1</sup>, N. Dubrovinskaia<sup>1</sup>

<sup>1</sup>Universität Bayreuth, Bayreuth, Germany

In a science fiction novel published by Jules Verne in 1864 travelers to the center of the Earth encountered “crystals...like globes of light”. One hundred and fifty years later, studies of crystals compressed to enormous pressure exceeding millions of atmospheres are shining light on the inner Earth.

The Earth’s deep interior is largely inaccessible (the deepest hole at the Kola peninsula in Russia is of about 12 km depth, only a small fraction of a percent of the Earth’s radius), and consequently most of our understanding is based on indirect inferences. These include the average chemical composition of the solar system, the chemical composition of rocks near the Earth’s surface, geophysical measurements of the Earth’s density and of the seismic wave-velocity distribution, and laboratory studies of the state and properties of materials at high pressures and temperatures.

A diamond anvil cell (DAC) is the primary tool for high-pressure and high-temperature mineral studies. Samples of less than 0.1 mm across are compressed between the tips of gem-quality diamonds. X-rays and lasers are fired through the diamond anvils at the samples to heat them and investigate their chemical and phase state, and their properties.

Laser heating techniques in diamond anvil cells cover a wide pressure-temperature range extending values characteristic for the Earth’s core (360 GPa and above 5000 K). However, until recently, existing DAC laser-heating systems could not be used for structural X-ray diffraction studies aimed at structural solutions and refinements. The reason is that in existing DAC laser-heating facilities the laser beam enters the cell and hits the crystal at a fixed angle. A partial rotation of the DAC, as required in monochromatic structural X-ray diffraction experiments, results in a loss of the target crystal from the laser beam. If in the meanwhile the powerful laser light starts to scatter in arbitrary directions by the diamond anvils, it may be even dangerous. In order to overcome this problem we have developed a portable laser heating system, implemented it at various diffraction beam lines, and applied it for investigations of a number of oxides, silicates, carbonates, and alloys which are expected to be found in Earth’s mantle and core. Traveling along the thermodynamic path through the inner Earth conditions we and colleagues made several unexpected findings which affect our understanding of how our planet is functioning, how processes in the interiors are linked to the events on the earth surfaces, including global climatic changes and mass extinctions.



*Institute of Geoecology and Geoinformation,  
Adam Mickiewicz University in Poznań, Poland*

**Thursday, 7 September 2017, 8.00, Room 2.64**

### **Biographical sketch**

Dr Mirostaw Makohonienko obtained his Ph.D. degree in Earth Sciences from Nicolaus Copernicus University in Toruń, Poland in 1998. He is geologist and archaeologist specialised in Quaternary palaeoecology, biogeography and environmental archaeology. His main interest concerns history of vegetation changes, natural and cultural landscape development, man-environment interactions. In 1992-1993 he obtained research scholarship in the Quaternary Department of Lund University, Sweden. In 1994 he worked at Christian Albrechts University in Kiel, Germany in the Institute of Pre- and Protohistoric Archaeology. In the years 1998-2001 he obtained scholarship at Kyoto University and International Research Center for Japanese Studies in Kyoto, Japan. In 2005 was a research fellow in IRCJS under the guidance of Professor Yoshinori Yasuda. In that time he participated in numerous expeditions in East Asia – in China, Korea and Japan. His habilitation thesis written in 2009 concerned natural and anthropogenic vegetation changes in north-east China during Holocene. He is author or co-author of over 120 scientific articles and chapters in monographs, author of four books and co-editor of several monographs. Co-founder of the Association of Environmental Archaeology in Poland, twice elected as its president. He organized over 20 domestic and several international conferences dedicated to Quaternary environmental changes. Presently, he has position of professor at Adam Mickiewicz University in Poznań. Head of the Department of Quaternary Geology and Palaeogeography and deputy-director of the Institute of Geoecology and Geoinformation at the Faculty of Geographical and Geological Sciences.

## Meteorite Morasko – the largest iron meteorite shower in Central Europe

Mirosław Makohonienko<sup>1</sup>, Krzysztof Pleskot<sup>1</sup>, Andrzej Muszyński<sup>2</sup>,

Witold Szczuciński<sup>2</sup>, Małgorzata Bronikowska<sup>2</sup>

<sup>1</sup>Institute of Geoecology and Geoinformation, Adam Mickiewicz University in Poznań, Poland (speaker)

<sup>2</sup>Institute of Geology, Adam Mickiewicz University in Poznań, Poland

The Morasko Hill (Góra Moraska) located at the northern fringe of Poznań city, is the highest elevation (153.75 m a.s.l.) in the region of Central Great Poland. Its main landscape features were formed during the last cold epoch called Vistulian glaciation. A unique phenomenon of the Morasko Hill have been discussed since 1914 when dr Cobliner reported the first findings of extraterrestrial matter, consisting of four iron meteorites discovered during digging of military trenches. The weight of biggest meteorite was 77.5 kg, the next one 4.2 kg and the other two meteorites 3.5 kg each. Since that time, numerous iron meteorites have been found in the area, distributed along NE to SW transect. The total weight of reported meteorite findings from Morasko Hill is estimated to around 1,500 kg. The biggest specimen, found in 2012, was over 261 kg and is the biggest meteorite found in Poland.

In 1957, for the first time the meteorite findings were associated with the presence of regular round depressions on the northern slope of Morasko Hill, interpreted as meteorite craters. The Morasko strewn field comprises seven impact craters. Their diameters range from 20 to almost 100 m, some of them are permanently or temporarily filled with water. The presence both of extraterrestrial matter and morphological effects of meteorite fall is very rare, documented so far in less than 20 sites in the world. Morasko Hill provided record of the largest iron meteorite shower in Central Europe. The impact has been dated to the mid Holocene, around 5,000 years ago, i.e. during the Neolithic times, when the area was settled by societies of Funnel Beaker Culture.

Numerical modelling determined the preatmospheric parameters of the Morasko meteoroid. The entry mass was around 600 to 1,100 tons and its initial radius was about 2-4 m. The velocity range was between 16 and 18 km/s, and the trajectory angle between 30 and 40°. Such entry velocities and trajectory angles do not deviate from typical values for near-Earth asteroids, although the initial mass determined can be considered as small. The airburst altitude was about 8 km above the Earth surface, and its energy was estimated to be about 7-9 kilotons. The total energy of the Morasko event did not exceeded 30 kilotons. The formation of the biggest Morasko crater is estimated for the iron projectile parameters as follows: impact velocity 6.07 km/s and projectile radius of 1.54 m. The peak shock pressure resulting from such conditions was about 60 GPa and it occurred at the contact point between the projectile and the target. The volume of target material shocked above 5 GPa during this crater formation was about 1,570 m<sup>3</sup>, while only about 1m<sup>3</sup> is shocked above 30 GPa. Such results presume that it would be extremely difficult



to identify shock indicators in the Morasko impact area. The calculations related to the shock wave propagation indicates that environmental consequences of this impact event are highly localized, while any earthquakes and long-term consequences can be considered as impossible. Palaeoenvironmental studies carried out on lake deposits in the region seem to confirm the modelling indications. In the light of sedimentological and palynological data the regional environments did not undergo substantial transformations of the landscape.

Morasko impact belongs to very rare impact sites preserved in soft sedimentary rocks. In 1976, the Morasko Hill with craters and fragments of oak-hornbeam forest were protected as natural preserve, and classified at the list of national geosites. Mineralogical analyses of the Morasko extraterrestrial matter provided two new minerals – i.e. Moraskoite  $\text{Na}_2\text{Mg}(\text{PO}_4)\text{F}$  and Czochralskiite  $\text{Na}_4\text{Ca}_3\text{Mg}(\text{PO}_4)_4$ .



## Programme overview • Chairs & Speakers

Sunday, 3 September 2017		Monday, 4 September 2017			
	Room 2.64				
	8.45 - 9.00				
	Opening Ceremony				
	9.00 - 10.00				
	L. Dubrovinsky				
	Plenary Lecture 1 Ho-Kwang (David) Mao				
	Room 2.64	Room 2.61	Room 3.65	Room 2.62	
	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	
	S 1	S 2	S 3	S 6	
	K. F. Dziubek	M. Szafranski	G. Garbarino	R. Ahuja	
	M. Taravillo Corralo		G. Weck		
	W. Grochala	L. Mañosa	G. Weck	C. Jin	
	D. Santamaría-Pérez	D. Pinkowicz	D. Paliwoda	S. Medvedev	
	D. Sclta	X. Cao	K. Fuchizaki	V. Svitlyk	
	M. Peña-Álvarez	S. Klotz	C. G. Pruteanu	F. Capitani	
	U. Schwarz		S. Ayrihac	Y. Qi	
				G. Garbarino	
	Room 2.64	Room 2.61	Room 3.65	Room 2.62	
	14.00 - 16.00	14.00 - 16.00	14.00 - 16.00	14.00 - 16.00	
	S 5	S 4	S 7	S 8	
	J. Haines	U. Schwarz	I. Grzegory	B. Zakharov	
	N. Dubrovinskaia				
	C. Pépin	I. Loa	S. J. Rzoska	K. Dziubek	
	A. Grzelak	M. Marqués	S. Kralj	D. Zimmer	
	D. Laniel	M. Hanfland	M. Śmiechowski	F. Montisci	
	X. Li	M. Ceppatelli	J. Proctor	M. Marchivie	
	H. Vondracek	B. Sadovyi		M. Meyer	
	C. Meng				
	Room 2.57	16.30 - 18.30			
	16.00 - 18.00	16.30 - 18.30			
Room 2.57 18.00 - 19.00	EHPRG Committee Meeting	Poster Session 1 Level 0 odd numbers (P1, P3, P5...P91)			
Welcome Reception					



# Programme overview • Chairs & Speakers

Tuesday, 5 September 2017				Wednesday, 6 September 2017		
Room 2.64				Room 2.64		
9.00 - 10.00				9.00 - 10.00		
L. Dubrovinsky				L. Smeller		
Plenary Lecture 2 Natalia Dubrovinskaja				Plenary Lecture 3 Chris W. Michiels		
Room 2.62	Room 2.61	Room 3.65	Room 2.64	Room 3.65	Room 2.62	Room 2.64
10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30
<b>S 9</b>	<b>S 10</b>	<b>S 11</b>	<b>S 12</b>	<b>S 17</b>	<b>S 18</b>	<b>S 20</b>
K. V. Kamenev	G. Weck	L. Barbour	F. Fabbiani	L. Dubrovinsky	L. Smeller	B. Lavina
	M. Guthrie	M. Aniola	C. Hejny	S. McWilliams		
R. Khasanov	B. Haberl	S. Moggach	N. Casati	A. Lazicki	H. R. Kalbitzer	R. Boehler
G. Garbarino	R. S. McWilliams	W. Li	A. Pakhomova	D. Kraus	A. Lazarev	M. Guthrie
T. Plisson	J. M. Braun	S. Sobczak	B. Zakharov	A. L. Coleman	N. J. Brooks	M. Stekiel
J. Graf		D. Orlikowski	P. A. Guřka	N. J. Hartley	I. B. Rietveld	G. Aprilis
C. McMonagle		L. Barbour	N. Funnell	F. M. Shakhov		I. Ohira
				X. P. Zhang		
13.30 - 14.00						
EHPRG Group Photo						
Room 3.65	Room 2.61	Room 2.64	Room 2.62	Room 2.64		
14.00 - 16.00	14.00 - 16.00	14.00 - 16.00	14.00 - 16.00	12.30 - 14.00		
<b>S 13</b>	<b>S 14</b>	<b>S 15</b>	<b>S 16</b>	EHPRG General Assembly		
S. Klotz	S. (Montu) Saxena	K. Wang	R. Martořak			
A. Pakhomova	C. R. S. Haines	J. Haase	R. Ahuja	15.30 - 20.00		
C. Bull	N. Tateiwa	A. Kaminska	S. Scandolo	Excursions		
G. Garbarino	I. Yahniuk	D. Errandonea	A. Kvashnin			
C. Tulk	O. Matthies	G. Spiekermann	D. Kurzydowski			
F. Alabarse	J. Contreras-García	V. Monteseguro-Padrón				
		P. Rosa				
		M. A. Hakeem				
17.30 - 19.30						
Demonstration 1/2 h						
Open lecture Leonid Dubrovinsky Auditorium of AMU, Wieniawskiego Street 1						



## Programme overview • Chairs & Speakers

Thursday, 7 September 2017			Friday, 8 September 2017		
Room 2.64					
8.00 - 10.00					
Special Session: Morasko Meteorite Reserve Miroslaw Makohonienko			Room 2.64		
			9.00 - 10.00		
			S. A. T. Redfern		
			Plenary Lecture 5 Przemyslaw Dera		
Room 2.62	Room 3.65	Room 2.64	Room 2.62	Room 3.65	Room 2.64
10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30	10.30 - 12.30
S 22	S 23	S 24	S 26	S 27	S 28
S. Rzoska	C. Pulham	P. Dera	G. K. Rozenberg	S. Scandolo	S. A. T. Redfern
	W. Luo	Y. Lee	D. Pinkowicz		
A. Wesolowska	Y. Ding	M. Santoro	D. I. Khomskii	I. Errea	Y. Lee
Y. Zhang	M. Tkacz	P. Botella Vives	G. R. Hearne	M. Martinez-Canales	B. Lavina
J. Nasitowska	C. Ridley	J. Kim	S. V. Ovsyannikov	S. Biswas	W. Paszkowicz
E. Malinowska-Pańczyk	Y. Qi	J. Gawraczyński	T. Meier	R. Martoňák	F. Maeda
L. G. Fidalgo		J. Angel Sans	M. W. Kupa	W. Knap	M. Núñez-Valdez
J. A. Saraiva					
Room 2.57					
12.30-14.30					
Special Session: Women Under Pressure gathering			Room 2.64		
Room 2.64			12.40 - 13.00		
14.00 - 15.00			Closing Ceremony		
C. Pulham					
Plenary Lecture 4 Elena Boldyreva					
15.00 - 17.00					
Poster Session 2 Level 0 even numbers (P2, P4, P6...P90)					
19.00 - 23.00					
Gala Dinner Concordia Design, Zwierzyniecka Street 3					





## Scientific programme • Monday, 4 September 2017

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- 8.45-9.00            [Opening Ceremony](#)  
Room:                [2.64](#)
- 9.00-10.00         [PL 1 – Plenary Lecture 1](#)  
Room:                [2.64](#)  
Chair:                Leonid Dubrovinsky (Bayreuth/Germany)
- Superoxidation, hydrogen generation, and new paradigm of the deep Earth  
**Ho-Kwang (David) Mao** (Shanghai/China; Washington/US), Q. Hu
- 10.00-10.30         [Coffee Break](#)
- 10.30-12.30         [S 1 – High-pressure chemistry](#)  
Room:                [2.64](#)  
Chairs:               Kamil F. Dziubek (Fiorentino/Italy), Mercedes Taravillo Corralo (Madrid/Spain)
- 10.30-11.30         Silverish squeezing: lessons from high-pressure studies of the  
IL 1.1                compounds of Ag(I), Ag(II) and Ag(III)  
**Wojciech Grochala** (Warsaw/Poland), A.Grzelak, J. Gawraczyński, M. Derzsi, T. Jaroń, D. Kurzydłowski, P.J. Leszczyński, Z. Mazej, M. Somayazulu, V.B. Prakapenka, V. Struzhkin
- 11.30-11.45         Exploring the chemical reactivity of carbon dioxide at high-pressure  
IO 1.1                and high-temperature conditions  
**David Santamaría-Pérez** (Valencia/Spain), A. Kavner, S. Palaich, C. McGuire, A. Mahkluf, C.E. Manning, C.A. Tulk, J. Molaison, M. Guthrie, A. Doran, M. Kunz, C. Popescu, T. Marqueño, J. Ruiz-Fuertes, D. Errandonea, R. Chulia, D. Martinez-Garcia, J. Pellicer-Porres, S. MacLeod, D. Daisenberger, J.L. Jorda, F. Rey
- 11.45-12.00         High-pressure chemistry of red and black phosphorus with NH<sub>3</sub>  
IO 1.2                **Demetrio Scelta** (Sesto/Italy), A. Baldassarre, M. Serrano Ruiz, A. Cairns, A. Marchuk, S. Vogel, W. Schnick, R. Bini, M. Peruzzini, M. Ceppatelli



## Scientific programme • Monday, 4 September 2017

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- 12.00-12.15  
IO 1.3      Linear and cyclic phenyl oligomers: effect of cyclic configuration on the high-pressure phenyl products  
[Miriam Peña-Álvarez](#) (Edinburgh/United Kingdom; Madrid/Spain), S. Fanetti, N. Falsini, J.J. Casado, J.T. López Navarrete, V.G. Baonza, R. Bini, M. Taravillo, M. Citroni
- 12.15-12.30  
IO 1.4      High-pressure synthesis of intermetallic p-block superconductors  
[Ulrich Schwarz](#) (Dresden/Germany), A. Wosylus, K. Meier, S. Tence, K. Guo, R. Castillo, W. Schnelle, H. Rosner, A. Ormeci, A. Baranov, R. Cardoso-Gil, M. Bobnar, Y. Grin
- 10.30- 12.30  
Room:      **S 2 – New phenomena at high pressure**  
Chair:      **2.61**  
                 Marek Szafrński (Poznań/Poland)
- 10.30-11.15  
IL 2.1      Materials with giant mechanocaloric effects: Cooling by strength  
[Luís Mañosa](#) (Barcelona/Spain), A. Planes
- 11.15-11.40  
IO 2.1      Pressure effects in the family of octacyanonitobate-based molecular magnets  
[Dawid Pinkowicz](#) (Cracow/Poland), P. Konieczny, M. Rams, M. Mišek, K. Kamenev, H. Tomkowiak, A. Katrusiak
- 11.40-12.05  
O 2.1      Pressure-dependent Hugoniot elastic limit of polycrystalline YAG transparent ceramics  
[Xiuxia Cao](#) (Mianyang/China), Y. Yu, C. Meng, X. Li, J. Qi
- 12.05-12.30  
O 2.2      Bulk modulus and equation-of-state of ice VII and VIII by high pressure neutron scattering  
[Stefan Klotz](#) (Paris/France), K. Komatsu, H. Kagi, K. Kunc, A. Sano-Furukawa, S. Machida, T. Hattori
- 10.30-12.30  
Room:      **S 3 – Amorphous materials and liquids under pressure**  
Chair:      **3.65**  
                 Gaston Garbarino (Grenoble/France),  
                 Gunnar Weck (Bruyères-le-Châtel/France)



- 10.30-11.10  
IL 3.1      Melting curve and structure of simple fluids probed by X-ray diffraction  
[Gunnar Weck](#) (Bruyères-le-Châtel/France), G. Garbarino, F. Datchi, S. Ninet, D. Spaulding, J.A. Queyroux, T. Plisson, P. Loubeyre, M. Mezouar
- 11.10-11.30  
IO 3.1       $sp^3$ -Carbon nanomaterials synthesized at high pressure  
[Damian Paliwoda](#) (Bethlehem/US), M. Baldini, S. Najiba, C. Liu, Y. Fei, K. Landskron
- 11.30-11.50  
O 3.1      Liquid—liquid transition in  $Ge_4$   
[Kazuhiro Fuchizaki](#) (Matsuyama; Kashiwa/Japan), H. Nishimura, T. Sakagami, T. Hase, H. Iwayama, N. Hamaya, H. Saitoh
- 11.50-12.10  
O 3.2      Why dense mixtures are different: aqueous solutions of methane and nitrogen  
[Ciprian G. Pruteanu](#) (Edinburgh/United Kingdom), W.F. Kuhs, M. Mlinarevic, T. Mlinarevic, J.S. Loveday
- 12.10-12.30  
IO 3.2      Anomalous sound velocity in liquid heavy alkali metals at extreme conditions  
[Simon Ayrinhac](#) (Paris/France), M. Gaunthier, M. Morand, F. Decremps
- 10.30-12.30  
Room:  
Chair:      **S 6 – Superconductivity under high pressure: experiment and theory 2.62**  
Rajeev Ahuja (Uppsala/Sweden)
- 10.30-11.15  
IL 6.1      Pressure induced superconductivity in spin orbital coupling system  
[Changqing Jin](#) (Beijing/China)
- 11.15-11.30  
O 6.1      Pressure-induced superconductivity in the pyrite phase of palladium diselenide  
[Sergey Medvedev](#) (Dresden/Germany), M. ElGhazali, P. Naumov, H. Mirhosseini, L. MÜchler, C. Felser



## Scientific programme • Monday, 4 September 2017

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- 11.30-11.45  
O 6.2      Kinetically stabilized order and phase separation in superconducting  $\text{Cs}_x\text{Fe}_{2-y}\text{Se}_2$  at high pressure  
[Volodymyr Svitlyk](#) (Grenoble/France), E. Pomjakushina, A. Krzton-Maziopa, K. Conder, M. Mezouar
- 11.45-12.00  
O 6.3      Spectroscopic evidence of a new energy scale for superconductivity in  $\text{H}_3\text{S}$   
[Francesco Capitani](#) (Saint-Aubin/France), B. Langerome, J.-B. Brubach, P. Roy, A. Drozdov, M. Eremets, E. Nicol, J. Carbotte, T. Timusk
- 12.00-12.15  
O 6.4      Topological quantum phase transition and superconductivity induced by pressure in the bismuth tellurohalide BiTeI  
[Yanpeng Qi](#) (Dresden/Germany), W. Shi, P.G. Naumov, N. Kumar, R. Sankar, W. Schnelle, C. Shekhar, F.C. Chou, C. Felser, B. Yan, S.A. Medvedev
- 12.15-12.30  
O 6.5      Iron-based superconductivity extended to the novel hydride  $\text{LaFeSiH}$   
[Gaston Garbarino](#) (Monserato/Italy), F. Bernardini, A. Sulpice, M. Núñez-Regueiro, E. Gaudin, B. Chevalier, A. Cano, S. Tencé
- 14.00-16.00  
Room: [2.61](#)  
Chair: [Ulrich Schwarz](#) (Dresden/Germany)  
**S 4 – Elements and binary alloys under pressure: structural and electronic transformations**
- 14.00-14.40  
IL 4.1      Host-guest phases and their properties: from elements to alloys  
[Ingo Loa](#) (Edinburgh/United Kingdom)
- 14.40-15.00  
IO 4.1      Alkali metal incommensurate phases: stability and electronic structure  
[Miriam Marqués](#) (Edinburgh/United Kingdom), G. Woolman, V. Naden-Robinson, I. Loa, G.J. Ackland, A. Hermann
- 15.00-15.20  
IO 4.2      Structures of simple elements by single crystal diffraction  
[Michael Hanfland](#) (Grenoble/France)



## Scientific programme • Monday, 4 September 2017

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- 15.20-15.40  
O 4.1      The mechanism of the A7 to sc phase transition in black phosphorus  
Matteo Ceppatelli (Sesto/Italy), D. Scelta, A. Baldassarre, M. Serrano Ruiz, K. Dziubek, A. Cairns, M. Peruzzini, R. Bini
- 15.40-16.00  
O 4.2      Extreme HT-HP conditions for activation of noticeable oxygen diffusion in GaN  
Bogdan Sadovyi (Warsaw/Poland), A. Nikolenko, J.L. Weyher, S. Porowski, I. Petrusha, V. Turkevich, I. Karbovnyk, V. Kapustianyk, I. Grzegory
- 12.30-14.00      **Lunch Break**
- 14.00-16.00  
Room:      **S 5 – Materials chemistry at high pressure**  
              **2.64**  
Chairs:      Julien Haines (Montpellier/France), Natalia Dubrovinskaia (Bayreuth/Germany)
- 14.00-14.20  
IO 5.1      Synthesis of FeH<sub>5</sub>: dense atomic metal hydrogen stabilized by Fe  
Charles Pépin (Arpajon/France; Lausanne/Switzerland), G. Geneste, A. Dewaele, M. Mezouar, P. Loubeyre
- 14.20-14.40  
O 5.1      Unprecedented crystal structures of HP polymorphs of AgO and AgF<sub>2</sub>  
Adam Grzelak (Warsaw/Poland), J. Gawracyński, T. Jaroń, D. Kurzydłowski, Z. Mazej, P.J. Leszczyński, V.B. Prakapenka, M. Derzi, M. Somayazulu, V. Struzhkin, W. Grochala
- 14.40-15.00  
O 5.2      Unexpected chemistry of hydronitrogen compounds under pressure: The case of N<sub>2</sub>(H<sub>2</sub>)<sub>2</sub>  
Dominique Laniel (Arpajon/France), V. Svitlyk, G. Weck, P. Loubeyre
- 15.00-15.20  
O 5.3      High purity MoN<sub>2</sub> synthesized by high pressure ion exchange reaction method  
Xuhai Li (Mianyang/China), L. Xu, L. Liu, C. Meng, X. Cao, Y. Wang, Q. Wu
- 15.20-15.40  
O 5.4      The H-bond dynamics of aqueous solutions under high pressure  
Hendrik Vondracek (Bochum/Germany), L. Knake, I. Kolling, G. Schwaab, M. Havenith



## Scientific programme • Monday, 4 September 2017

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- 15.40-16.00  
O 5.5      Reaction synthesis of  $\text{Mo}_2\text{C}$  by shock-wave compression method  
[Chuanmin Meng](#) (Mianyang/China), X. Li, L. Xu, L. Liu, Y. Wang,  
X. Cao
- 14.00-16.00      [S 7 – Critical and supercritical fluids under pressure](#)  
Room: [3.65](#)  
Chair: Izabella Grzegory (Warsaw/Poland)
- 14.00-14.40      Critical liquids under pressure  
IL 7.1      [Sylwester J. Rzoska](#) (Warsaw/Poland), A. Drozd-Rzoska
- 14.40-15.20      Supercooled soft nanocomposites  
IL 7.2      [Samo Kralj](#) (Ljubljana/Slovenia), Z. Kutnjak, S. Rzoska
- 15.20-15.40      Terahertz spectroscopy and the hydrogen bond network of  
IO 7.1      supercritical water  
[Maciej Śmiechowski](#) (Gdańsk/Poland), D. Marx
- 15.40-16.00      Crossover between liquid-like and gas-like behaviour in  $\text{CH}_4$  at 400 K  
O 7.1      [John E. Proctor](#) (Manchester/United Kingdom), D. Smith, M.A.  
Hakeem, P. Parisiades, H.E. Maynard-Casely, D. Foster, D. Eden,  
D.J. Bull, A.R.L. Marshall, A.M. Adawi, R. Howie, A. Sapelkin,  
V.V. Brazhkin
- 14.00-16.00      [S 8 – High pressure structural analysis and \(meta\)data deposition](#)  
Room: [2.62](#)  
Chair: Boris Zakharov (Novosibirsk/Russia)
- 14.00-14.45      Collect, protect, share and use. Behind the barricades of data  
IL 8.1      revolution in high pressure research  
[Kamil F. Dziubek](#) (Fiorentino/Italy)
- 14.45-15.00      Pressure-induced phase transitions in copper sulfides  
O 8.1      [Dominik Zimmer](#) (Frankfurt am Main/Germany), W. Morgenroth,  
J. Ruiz-Fuertes, E. Haussühl, L. Bayarjargal, D. Santamaría-Pérez,  
B. Winkler



## Scientific programme • Monday, 4 September 2017

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- 15.00-15.15  
O 8.2      Weak donor-acceptor intermolecular interactions under pressure:  
the  $\text{NO}_2 \cdots \text{NO}_2$  case  
[Fabio Montisci](#) (Bern/Switzerland), A. Lanza, N. Casati, P. Macchi
- 15.15-15.30  
O 8.3      Spin Crossover molecular complexes behavior under pressure:  
contribution of the structural approach  
[Mathieu Marchivie](#) (Pessac/France), E. Tailleux, P. Rosa, S. Matar,  
V. Legrand, J.P. Itié, P. Guionneau
- 15.30-16.00  
IO 8.1      HP experiments and data reduction with CrysAlisPro  
[Mathias Meyer](#) (Wrocław/Poland)
- 16.00-16.30      [Coffee Break](#)
- 16.30-18.30      [Poster Session 1](#)  
[Level 0](#)



## Scientific programme • Tuesday, 5 September 2017

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- 9.00-10.00      [PL 2 – Plenary Lecture 2](#)  
Room:            [2.64](#)  
Chair:            Leonid Dubrovinsky (Bayreuth/Germany)
- Structural studies taken to the extreme  
**Natalia Dubrovinskaia** (Bayreuth/Germany), L. Dubrovinsky
- 10.00-10.30      [Coffee Break](#)
- 10.30-12.30      [S 9 – High-pressure instrumentation](#)  
Room:            [2.62](#)  
Chair:            Konstantin V. Kamenev (Edinburgh/United Kingdom)
- 10.30-11.20      High pressure research using muons  
IL 9.1            [Rustem Khasanov](#) (Villigen/Switzerland)
- 11.20-11.45      High pressure developments at the ESRF: present status and  
O 9.1            perspectives  
[Gaston Garbarino](#) (Grenoble/France), J. Jacobs
- 11.45-12.00      Magnetic sensing at high pressure in the diamond anvil cell using  
O 9.2            NV-centers implanted at the diamond tip  
[Thomas Plisson](#) (Arpajon/France), M. Lesik, L. Toraille, J. Renaud,  
O. Salord, A. Delobbe, L. Rondin, P. Loubeyre, J.-F. Roch
- 12.00-12.15      Squeezing the most data out of your high-pressure experiment  
O 9.3            [Juergen Graf](#) (Geesthacht/Germany), M. Ruf, T. Stuerzer, H. Ott,  
M. Adam
- 12.15-12.30      A moderate pressure cell for the Small Molecule Beamline I19 at  
O 9.4            Diamond Light Source  
[Charlie McMonagle](#) (Edinburgh/United Kingdom), M.R. Warren,  
D.R. Allan, K.V. Kamenev, S. Parsons, P.A. Wright, S.A. Moggach





## Scientific programme • Tuesday, 5 September 2017

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- 10.30-12.30      [S 10 – New techniques at large scale facilities](#)  
Room:            [2.61](#)  
Chairs:           Gunnar Weck (Arpajon/France), Malcolm Guthrie (Lund/Sweden)
- 10.30-11.20      High pressure neutron scattering in a diamond anvil cell at Oak  
IL 10.1           Ridge National Laboratory  
[Bianca Haberl](#) (Oak Ridge/US), J.J. Molaison, R. Boehler
- 11.20-12.10      Phase transformations and transport properties at high pressure and  
IL 10.2           temperature from dynamic measurements under static compression  
[R. Stewart McWilliams](#) (Edinburgh/United Kingdom),  
N. Gomez-Perez, H.B. Scott, J. Meza-Galvez, J.F. Rodriguez, T. Kimura,  
M.F. Mahmood, H.P. Liermann, Z. Konopkova, A.F. Goncharov
- 12.10-12.30      Pressure-induced insulator-to-metal transition in VO<sub>2</sub> studied by  
O 10.1           near-infrared pump – mid-infrared probe spectroscopy  
[Johannes M. Braun](#) (Dresden/Germany), H. Schneider, M. Helm,  
R. Mirek, L.A. Boatner, R.E. Marvel, R.F. Haglund, A. Pashkin
- 10.30-12.30      [S 11 – Porous framework under pressure](#)  
Room:            [3.65](#)  
Chairs:           Len Barbour (Matieland/RSA), Michalina Aniola (Poznań/Poland)
- 10.30-11.10      Pressure and temperature-induced phase transitions,  
IL 11.1           piezochromism, NLC behaviour and Jahn–Teller pressure switching  
in a one-dimensional Cu-based framework  
[Stephen A. Moggach](#) (Edinburgh/United Kingdom), C. McMonagle,  
D.R. Allan, E.K. Brechin, P. Comar, G. Nichol, S. Parsons, S. Sanz
- 11.10-11.35      Influences of chemical bonding in mechanical properties & phase  
IO 11.1           transitions of metal-organic frameworks  
[Wei Li](#) (Wuhan/China)
- 11.35-11.50      Negative volume compression revealed by X-Ray diffraction  
O 11.1           [Szymon Sobczak](#) (Poznań/Poland), A. Katrusiak
- 11.50-12.05      Rapid compression of granular systems using atomistic molecular  
O 11.2           dynamic simulations  
[Daniel Orlikowski](#) (Livermore/US)
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## Scientific programme • Tuesday, 5 September 2017

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- 12.05-12.30  
IL 11.2      Tools for studying the effects of gas pressure on porous materials in the solid state  
[Len Barbour](#) (Matieland/RSA)
- 10.30-12.30  
Room:      [S 12 – High pressure crystallographic studies](#)  
2.64  
Chairs:      Francesca Fabbiani (Göttingen/Germany), Clivia Hejny (Innsbruck/Austria)
- 10.30-11.10  
IL 12.1      Chemistry at work under high pressure  
[Nicola Casati](#) (Villigen/Switzerland), T. Poreba, A. Kleppe, A. Jephcoat, P. Macchi
- 11.10-11.30  
IO 12.1      Pentacoordinated silicon in the high-pressure polymorph of danburite  
[Anna Pakhomova](#) (Hamburg/Germany), E. Bykova, M. Bykov, K. Glazyrin, B. Gasharova, H.-P. Liermann, M. Mezouar, L. Gorelova, S. Krivovichev, L. Dubrovinsky
- 11.30-11.50  
IO 12.2      Application of high pressures for understanding mechanical phenomena on solid-state transformations  
[Boris A. Zakharov](#) (Novosibirsk/Russia)
- 11.50-12.10  
O 12.1      Arsenolite and its helium clathrate: high pressure studies on cubic arsenic(III) oxide  
[Piotr A. Guńka](#) (Warsaw/Poland), K.F. Dziubek, A. Gładysiak, M. Dranka, J. Piechota, M. Hanfland, A. Katrusiak, J. Zachara
- 12.10-12.30  
O 12.2      High-pressure phase behaviour of ROY: a highly-compressible organic crystal  
[Nicholas Funnell](#) (Chilton/United Kingdom), C.L. Bull, C.J. Ridley
- 12.30-13.30      [Lunch Break](#)
- 13.30-14.00      [EGPRG Group Photo](#)



## Scientific programme • Tuesday, 5 September 2017

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- 14.00-16.00      [S 13 – Synchrotrons and neutron high-pressure facilities](#)  
Room:            [3.65](#)  
Chair:            Stefan Klotz (Paris/France)
- 14.00-14.25      The Extreme Conditions Beamline at PETRA III (DESY): outlook and  
IL 13.1            recent advances  
[Anna Pakhomova](#) (Hamburg/Germany), H.-P. Liermann, K. Glazyrin,  
E. Bykova, M. Bykov, W. Morgenroth, Z. Jenei, W. Evans, M. Wendt,  
S. Wenz, A. Ehnes, I. Schwark, J.-T. Roeh
- 14.25-14.50      Developments in the High Pressure User Programme at the ISIS  
IL 13.2            Neutron Source  
[Craig L. Bull](#) (Oxfordshire/United Kingdom), N.P. Funnell, C. Ridley
- 14.50-15.15      ID27, an advanced high flux XRD beamline for Science under  
O 13.1            extreme conditions: present and future  
[Gaston Garbarino](#) (Grenoble/France), M. Mezouar, V. Svitlyk,  
A. Cairns, D. Sifre, L. Henry, S. Bauchau
- 15.15-15.40      Recent developments of high pressure neutron scattering at SNAP  
O 13.2            [Chris Tulk](#) (Oak Ridge/US), A. dos Santos, J. Molaison, R. Boehler,  
B. Haberl, M. Guthrie
- 15.40-16.00      State of the art of Xpress – the high pressure diffraction beamline of  
O 13.3            the Elettra Synchrotron Trieste  
[Frederico Alabarse](#) (Trieste/Italy), B. Joseph, N.K. Varshney, G. Bais,  
G. Skerlj, M. Polentarutti, D.D. Sarma, A. Lausi
- 14.00-16.00      [S 14 – Pressure induced quantum criticality and novel emergent  
phases](#)  
Room:            [2.61](#)  
Chair:            Siddharth (Montu) Saxena (Cambridge/United Kingdom)
- 14.00-14.30      Direct control of quantum criticality in ferroelectrics  
IO 14.1            [Charles R. S. Haines](#) (Cambridge/United Kingdom), M.J. Coak, C. Liu,  
S.E. Rowley, S.S. Saxena



## Scientific programme • Tuesday, 5 September 2017

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- 14.30-15.00  
IO 14.2      Application of miniature high pressure cell for magnetic measurements to study of strongly correlated electron systems  
[Naoyuki Tateiwa](#) (Ibaraki/Japan)
- 15.00-15.20  
O 14.1      Influence of hydrostatic pressure on transition from topological insulator to band insulator phase in HgTe quantum well  
[Ivan Yahniuk](#) (Warsaw/Poland), G. Grabecki, M. Majewicz, J. Wróbel, T. Dietl, S. Krishtopenko, V. Gavrilenko, F. Teppe, S. Dvoretzky, N. Mikhailov, G. Cywiński, W. Knap
- 15.20-15.40  
O 14.2      Absent diamond-to- $\beta$ -Sn phase transition for carbon: quantum chemical topology approach  
[Olga Matthies](#) (Dresden/Germany), Y. Grin, M. Kohout
- 15.40-16.00  
O 14.3      Topological approaches to high pressure behavior  
[Julia Contreras-García](#) (Paris/France), J.A. Sans, M. Marqués, F.J. Manjón, P. Rodríguez-Hernández, A. Muñoz
- 14.00-16.00      [S 15 – High-pressure spectroscopy and structural studies of new materials](#)  
Room: [2.64](#)  
Chair: Kai Wang (Changchun/China)
- 14.00-14.30  
IL 15.1      Anvil cell NMR of solids  
[Juergen Haase](#) (Leipzig/Germany)
- 14.30-14.45  
IO 15.1      High pressure and time resolved studies of optical properties of nitride quantum structures - experimental and ab-initio analysis  
[Agata Kaminska](#) (Warsaw/Poland), P. Strak, K.P. Korona, E. Monroy, S. Krukowski



## Scientific programme • Tuesday, 5 September 2017

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- 14.45-15.00  
IO 15.2      Correlating changes induced by pressure in the structural and spectroscopic properties of  $\text{LaVO}_4$   
[Daniel Errandonea](#) (València/Spain), C. Ferrer-Roca, D. Martínez-García, J. Pellicer-Porres, J. Ruiz-Fuertes, U.R. Rodríguez-Mendoza, V. Lavín, P. Rodríguez-Hernández, A. Muñoz, A. Friedrich, W. Morgenroth, C. Popescu, M. Bettinelli
- 15.00-15.15  
O 15.1      Coordination and bond distances in compressed amorphous  $\text{GeO}_2$  up to 100 GPa by valence-to-core X-ray emission spectroscopy (vtc-XES)  
[Georg Spiekermann](#) (Potsdam; Hamburg/Germany), M. Harder, P. Zalden, C. Sahle, M. Wilke, N. Biedermann, C. Weis, W. Morgenroth, E. Kulik, N. Nishiyama, S. Petitgirard, H. Yavas, C. Sternemann
- 15.15-15.30  
O 15.1      High pressure characterization of the recent discovered phase of iron oxide: epsilon  $\text{Fe}_2\text{O}_3$   
[Virginia Monteseguro-Padrón](#) (Grenoble/France), J.Á. Sans-Tresserras, M. Gich, G. Garbarino, V. Cuartero-Yague, V. Cerantola, A. Muñoz-González, C. Popescu, M. Monte-Caballero
- 15.30-15.45  
O 15.2      (P,T,hv) phase diagram of spin crossover compounds  
[Patrick Rosa](#) (Pessac/France), M. Marchivie, P. Guionneau, B. Vignolle
- 15.45-16.00  
O 15.3      High pressure Raman, optical absorption and resistivity study of  $\text{SrCrO}_4$  up to 58 GPa  
[Malik A. Hakeem](#) (Greater Manchester/United Kingdom), J.E. Proctor, D.E. Jackson, J.J. Hamlin, D. Errandonea, M. Bettinelli
- 14.00-16.00  
Room:      **S 16 – Theoretical prediction of high-pressure phases**  
Chair:      **2.62**  
Roman Martoňák (Bratislava/Slovakia)
- 14.00-14.45  
IL 16.1      Structural phase transition in simple metals from ab initio calculations  
[Rajeev Ahuja](#) (Uppsala/Sweden)



## Scientific programme • Tuesday, 5 September 2017

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- 14.45-15.15  
IL 16.2      Microscopic mechanisms of the pressure-induced amorphization of  $\text{SiO}_2$   
[Sandro Scandolo](#) (Trieste/Italy), Y. Liang, C.R. Miranda
- 15.15-15.40  
IO 16.1      Computational search for novel materials for energy applications  
[Alexander Kvashnin](#) (Moscow/Russia), H.A. Zakaryan, A.R. Oganov, A.I. Samtsevich, Z. Allahyari
- 15.40-16.00  
O 16.1      Reactivity and magnetic properties of inorganic fluorides at large compression  
[Dominik Kurzydłowski](#) (Warsaw/Poland), P. Zaleski-Ejgierd, W. Grochala
- Venue:      [Open Lecture](#)  
[The Auditorium of Adam Mickiewicz University](#),  
Wieniawskiego 1, Poznań
- 17.30-18.00      Introductory presentation  
Life in extreme conditions: Can we colonize Venus and Mars?  
[Szymon Sobczak](#) (Poznań/Poland), [Michał Andrzejewski](#) (Bern/Switzerland)
- 18.00-19.30      Journey to the center of the Earth 150 years after Jules Verne: Science-not fiction  
[Leonid Dubrovinsky](#) (Bayreuth/Germany), N. Dubrovinskaia



- 9.00-10.00      [PL 3 – Plenary Lecture 3](#)  
Room:            [2.64](#)  
Chair:            László Smeller (Budapest/Hungary)
- Bacterial inactivation by high pressure treatment: recent insights and applications in food preservation  
**Chris W. Michiels** (Leuven/Belgium), A. Aertsen, E. Gayan
- 10.00-10.30      [Coffee Break](#)
- 10.30-12.30      [S 17 – Shock experiments and ultra-high pressure generation](#)  
Room:            [3.65](#)  
Chairs:           Leonid Dubrovinsky (Bayreuth/Germany), Stewart McWilliams (Edinburgh/United Kingdom)
- 10.30-11.10      Probing structure, phase boundaries and temperature of laser-compressed Pb  
IL 17.1            **Amy E. Lazicki** (Livermore/US)
- 11.10-11.30      Experimental investigation of diamond precipitation inside giant planets  
IO 17.1            **Dominik Kraus** (Dresden/Germany; Berkeley/US), J. Vorberger, A. Pak, N.J. Hartley, L.B. Fletcher, S. Frydrych, E. Galtier, E.J. Gamboa, D.O. Gericke, S.H. Glenzer, E. Granados, M.J. MacDonald, A.J. MacKinnon, E.E. McBride, I. Nam, P. Neumayer, M. Roth, A.M. Saunders, A.K. Schuster, P. Sun, T. van Driel, T. Doepfner, R.W. Falcone
- 11.30-11.45      A Comparison of the phase behaviour in dynamically and statically compressed antimony  
O 17.1            **Amy L. Coleman** (Edinburgh/United Kingdom), M.G. Gorman, R. Briggs, R.S. McWilliams, D. McGonegle, M. Stevenson, S. Macleod, S. Rothman, C.A. Bolme, G.W. Collins, J.H. Eggert, D.E. Fratanduono, R.F. Smith, E. Galtier, H.J. Lee, Z. Xing, J.S. Wark, E.E. McBride, M.I. McMahon



## Scientific programme • Wednesday, 6 September 2017

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- 11.45-12.00  
O 17.2      Hydrocarbons at extreme conditions  
[Nicholas J. Hartley](#) (Dresden-Rossendorf/Germany), J. Vorberger, A. Pak, T. Döppner, L.B. Fletcher, S. Frydrych, E. Galtier, E.J. Gamboa, D.O. Gericke, S.H. Glenzer, E. Granados, M.J. MacDonald, A.J. MacKinnon, E.E. McBride, I. Nam, P. Neumayer, K. Rohatsch, M. Roth, A.M. Saunders, A. Schuster, P. Sun, T. van Driel, R.W. Falcone, D. Kraus
- 12.00-12.15  
O 17.3      Boron doped diamond synthesized from detonation nanodiamond in a C-O-H fluid at high pressure and high temperature  
[Fedor M. Shakhov](#) (Saint-Petersburg/Russia), A.M. Abyzov, K. Takai
- 12.15-12.30  
O 17.4      Investigation of magnetically driven liner implosion on compact pulsed power generator  
[Xuping P. Zhang](#) (Mianyang/China), G.J. Wang, B.Q. Luo, F.L. Tan, J.H. Zhao, C.W. Sun, C.L. Liu
- 10.30-12.30  
Room:      [S 18 – High-pressure life and biosciences](#)  
Chair:      [2.61](#)  
                 László Smeller (Budapest/Hungary)
- 10.30-11.20  
IL 18.1      Excited states of proteins detected by high pressure NMR spectroscopy and their use for drug design  
[Hans Robert Kalbitzer](#) (Regensburg/Germany)
- 11.20-11.45  
O 18.1      Revisiting high-pressure acceleration of proteases: proteomics and high-pressure optical spectroscopy studies  
[Alexander Lazarev](#) (Massachusetts/US), G.B. Smejkal, V. Gross, P. Hains, K. Ashman, N. Curti
- 11.45-12.10  
O 18.2      Structure and mechanics of lipid membranes at high pressure  
[Nicholas J. Brooks](#) (London/ United Kingdom), N.L. McCarthy, H. Barriga, A.I.I. Tyler
- 12.10-12.30  
O 18.3      Mapping the phase behavior of the trimorphic prodrug L-tyrosine ethyl ester through measurement data and thermodynamics  
[Ivo B. Rietveld](#) (Mont Saint Aignan; Paris/France), B. Nicolai, A. Polian, M. Barrio, J.L. Tamarit





## Scientific programme • Wednesday, 6 September 2017

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- 10.30-12.30 S 20 – High-pressure studies in the Earth & planetary sciences  
Room: 2.64  
Chair: Barbara Lavina (Las Vegas/US)
- 10.30-11.00 Electrical resistivity of molten iron across the melting curve:  
IL 20.1 Implications for low conductivity in the outer core  
[Reinhard Boehler](#) (Washington/US), A. Basu, R. Boehler
- 11.00-11.30 Does the water molecule survive to 60 GPa?  
IL 20.2 [Malcolm Guthrie](#) (Lund/Sweden), R. Boehler, J.J. Molaison,  
B. Haberl, A. dos Santos, C.A. Tulk
- 11.30-11.50 High pressure elasticity of  $\text{FeCO}_3$ - $\text{MgCO}_3$  carbonates  
O 20.1 [Michal Stekiel](#) (Frankfurt am Main/Germany), T. Nguyen-Thanh,  
S. Chariton, C. McCammon, A. Bosak, W. Morgenroth, R. Luchitskaia,  
V. Milman, K. Refson, B. Winkler
- 11.50-12.10 Chemical interaction of iron with diamond anvils in pulsed and  
O 20.2 continuous wave laser heated diamond anvil cells  
[Georgios Aprilis](#) (Bayreuth/Germany), I. Kantor, I. Kuppenko,  
V. Cerantola, I. Collings, A. Pakhomova, R. Torchio, D. Vasiukov,  
S. Chariton, D. Simonova, C. McCammon, L. Dubrovinsky,  
N. Dubrovinskaia
- 12.10-12.30 Sound velocity and elasticity of  $\delta$ -(Al, Fe)OOH to lower mantle  
O 20.3 pressures  
[Itaru Ohira](#) (Tohoku/Japan), J.M. Jackson, W. Sturhahn,  
G.J. Finkelstein, S. Kamada, T. Kawazoe, F. Maeda, N. Hirao,  
S. Nakano, A. Suzuki, E. Ohtani
- 12.30-14.00 [EHPRG General Assembly](#)  
Room: 2.64
- 14.00-15.00 [Lunch Break](#)



## Scientific programme • Thursday, 7 September 2017

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- 08.00-10.00      **Special Session: Meteorite Reserve in Morasko - the largest iron meteorite shower in Central Europe**
- Mirosław Makohonienko** (Poznań/Poland), K. Pleskot, A. Muszyński, W. Szczuciński, M. Bronikowska
- 10.00-10.30      **Coffee Break**
- 10.30-12.30      **S 22 – Food science and technology**  
Room:            **2.62**  
Chair:            Sylwester Rzoska (Warsaw/Poland)
- 10.30-11.00      **New comments on the high pressure preservation of human milk**  
IL 22.1            **Aleksandra Wesołowska** (Warsaw/Poland), S.J. Rzoska, E. Rosiak, M.K. Borszewska-Kornacka
- 11.00-11.30      **Ultra high pressure processing to control bacterial spores for more gentle food preservation**  
IL 22.2            **Yifan Zhang** (Zurich/Switzerland), A. Waser, A. Mathys
- 11.30-11.45      **High pressure processing of vegetable juice: Evaluation of sublethal injured pathogen cells during long term storage using plate count methods and microscopy methods**  
O 22.1            **Justyna Nasiłowska** (Warsaw/Poland), B. Sokołowska, M. Fonberg-Broczek
- 11.45-12.00      **The effect of high pressure and subzero temperature on the microflora and selected components of human milk**  
O 22.2            **Edyta Malinowska-Pańczyk** (Gdańsk/Poland), D. Martysiak-Żurowska, M. Puta, B. Kusznerewicz
- 12.00-12.15      **Hyperbaric storage at room temperature of fresh Atlantic salmon (*Salmo salar*): microbial and physicochemical evaluation**  
O 22.3            **Liliana G. Fidalgo** (Aveiro/Portugal), A.T. Lemos, I. Delgadillo, J.A. Saraiva
- 12.15-12.30      **Bacillus subtilis endospore germination control by hyperbaric storage (food storage under pressure) – Carrot juice as case-study**  
O 22.4            **Jorge A. Saraiva** (Aveiro/Portugal), C.A. Pinto, M.D. Santos, L.G. Fidalgo, I. Delgadillo
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## Scientific programme • Thursday, 7 September 2017

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- 10.30-12.30      [S 23 – Energy materials under high pressure: experiment and theory](#)  
Room:            [3.65](#)  
Chairs:          Colin Pulham (Edinburgh/United Kingdom), Wei Luo (Uppsala/Sweden)
- 10.30-11.05      High pressure synchrotron study of electron correlated systems  
IL 23.1            [Yang Ding](#) (Beijing/China)
- 11.05-11.40      X-ray investigations of selected transition metals under high  
IO 23.1            pressure of hydrogen  
[Marek Tkacz](#) (Warsaw/Poland), M. Kuzovnikov, H. Meng
- 11.40-12.05      The effect of pressure on the structural and magnetic properties of  
O 23.1            some functional perovskites  
[Christopher Ridley](#) (Chilton/United Kingdom), N.P. Funnell,  
M. Capone, M. Guthrie, C.L. Bull
- 12.05-12.30      Superconductivity in alkaline earth metal-filled skutterudites  
O 23.2             $\text{Ba}_x\text{Ir}_4\text{X}_{12}$  (X = As, P)  
[Yanpeng Qi](#) (Yokohama/Japan), H. Lei, J. Guo, W. Shi, B. Yan,  
C. Felser, H. Hosono
- 10.30-12.30      [S 24 – Physics and transformations in compressed matter](#)  
Room:            [2.64](#)  
Chairs:          Przemysław Dera (Honolulu/Hawaii), Yongjae Lee (Seoul/Korea)
- 10.30-11.10      Sub-nano confined, dense simple molecular systems at high  
IL 24.1            pressures  
[Mario Santoro](#) (Sesto/Italy), R. Bini, M. Ceppatelli, K. Dziubek,  
F.A. Gorelli, M. Morana, D. Scelta, J.-M. Thibaud, J. Rouquette,  
P. Hermet, O. Cambon, F. Di Renzo, A. van der Lee, J. Haines
- 11.10-11.30      Single-walled carbon nanotubes shock-compressed to 0.5 MBar  
O 24.1            [Pablo Botella Vives](#) (Luleå/Sweden), X. Devaux, M. Dossot,  
V. Garashchenko, J.C. Beltzung, A.V. Soldatov



## Scientific programme • Thursday, 7 September 2017

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- 11.30-11.50  
O 24.2      Pressure dependent transport properties of TiZrNi quasicrystals  
Jaeyong Kim (Seoul/Korea), T. Lan Ahn Nghuyen, J. Won, S. Lee,  
S. Samanta, L. Wang
- 11.50-12.10  
O 24.3      Insight into high-pressure transformations of AgO, AgF and AgF<sub>2</sub>  
from Raman spectroscopy  
Jakub Gawraczyński (Warsaw/Poland), A. Grzelak, M. Derzsi,  
D. Kurzydłowski, T. Jaroń, A. Budzianowski, P. Leszczyński, Z. Mazej,  
V. Prakapenka, M. Somayazulu, V. Struzhkin, W. Grochala
- 12.10-12.30  
O 24.4      Hidden anomalous compressibility of  $\beta$ -Sb<sub>2</sub>O<sub>3</sub>  
Juan Angel Sans (Valencia/Spain), F.J. Manjón, A.L.J. Pereira,  
C. Popescu, A. Muñoz, P. Rodríguez-Hernández, J. Pellicer-Porres,  
V.P. Cuenca-Gotor, J. Contreras-García, V. Monteseguro-Padron,  
J. Ibañez
- 12.30-14.00  
Room:      **Special Session: “Women Under Pressure gathering”**  
2.57
- 12.30-14.00      **Lunch Break**
- 14.00-15.00  
Room:      **PL 4 – Plenary Lecture 4**  
2.64  
Chair:      Colin Pulham (Edinburgh/United Kingdom)
- Coordination and organic compounds at high pressures. Retrospect  
and challenges  
Elena Boldyreva (Novosibirsk/Russia)
- 15.00-17.00      **Poster Session 2**  
Level 0



## Scientific programme • Friday, 8 September 2017

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- 9.00-10.00      [PL 5 – Plenary Lecture 5](#)  
Room:            [2.64](#)  
Chair:            Simon A. T. Redfern (Cambridge/United Kingdom)
- Hypervalent penta-coordinated silicon and metastable phase transitions in silicates  
**Przemysław Dera** (Honolulu/Hawaii)
- 10.00-10.30      [Coffee Break](#)
- 10.30-12.30      [S 26 – Novel magnetic-electronic behavior at extreme P-T](#)  
Room:            [2.62](#)  
Chairs:           Gregory K. Rozenberg (Johannesburg/RSA), Dawid Pinkowicz (Cracow/Poland)
- 10.30-11.10      Correlated electrons, strong covalency and ligand holes, and their evolution under pressure  
IL 26.1            [Daniel I. Khomskii](#) (Koeln/Germany)
- 11.10-11.30      Spin crossover and charge gap resilience in ferrous spinels to a megabar  
IO 26.1            [Giovanni R. Hearne](#) (Johannesburg/RSA), W.M. Xu, S. Layek, D. Levy, J.-P. Itié, M.P. Pasternak, G.K. Rozenberg, E. Greenberg
- 11.30-11.50      Charge ordering in  $\text{Fe}_4\text{O}_5$   
IO 26.2            [Sergey V. Ovsyannikov](#) (Bayreuth/Germany), M. Bykov, E. Bykova, D.P. Kozlenko, A.A. Tsirlin, A.E. Karkin, V.V. Shchennikov, S.E. Kichanov, H. Gou, A.M. Abakumov, R. Egoavil, J. Verbeeck, C. McCammon, V. Dyadkin, D. Chernyshov, S. van Smaalen, L.S. Dubrovinsky
- 11.50-12.10      Magnetic flux amplification through Lenz lenses in toroidal diamond indenter cells: A new pathway to high pressure nuclear magnetic resonance  
IO 26.3            [Thomas Meier](#) (Bayreuth/Germany), S. Petitgirard, L. Dubrovinsky



## Scientific programme • Friday, 8 September 2017

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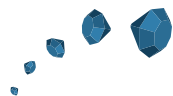
- 12.10-12.30  
IO 26.4      The development of high pressure ultrasonic setup to study strongly correlated systems  
[Michal W. Kopa](#) (Edinburgh/United Kingdom), C.J. Ridley, K.V. Kamenev, A.D. Huxley
- 10.30-12.30  
Room:      [S 27 – Structural phase transitions theory and experiment](#)  
Chair:      [3.65](#)  
Sandro Scandolo (Trieste/Italy)
- 10.30-11.10  
IL 27.1      Phase transitions from first-principles calculations and quantum symmetrization of hydrogen bonds in superconducting H<sub>3</sub>S  
[Ion Errea](#) (Bilbao/Spain), R. Bianco, F. Mauri
- 11.10-11.30  
O 27.1      The ground state of lithium  
[Miguel Martinez-Canales](#) (Edinburgh/United Kingdom), G. Ackland, M. Dunuwille, I. Loa, R. Zhang, S. Sinogeikin, W. Cai, S. Deemyad
- 11.30-11.50  
IO 27.1      Anharmonic effects in finite temperature B1-B2 phase transition of LiH  
[Sananda Biswas](#) (Trieste/Italy), I. Errea, F. Mauri, S. Scandolo
- 11.50-12.10  
IO 27.2      High-pressure phase diagram, structural transitions, and persistent non-metallicity of BaBiO<sub>3</sub>: theory and experiment  
[Roman Martoňák](#) (Bratislava/Slovakia), D. Ceresoli, T. Kagayama, Y. Matsuda, Y. Yamada, E. Tosatti
- 12.10-12.30  
IO 27.3      Pressure and temperature-driven phase transitions in Hg(Cd)Te quantum wells and bulk films  
[Wojciech Knap](#) (Montpellier/France; Warsaw/Poland), S.S. Krishtopenko, I. Yahniuk, S. Ruffenach, M. Marcinkiewicz, G. Cywinski, F. Teppe
- 10.30-12.30  
Room:      [S 28 – High pressure mineral physics and geochemistry](#)  
Chair:      [2.64](#)  
Simon A. T. Redfern (Cambridge/United Kingdom)
- 10.30-11.10  
IL 28.1      High-pressure chemistry of zeolites, MOFs, and clays  
[Yongjae Lee](#) (Seoul/Korea)
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## Scientific programme • Friday, 8 September 2017

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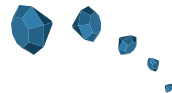
- 11.10-11.40  
IO 28.1 High-pressure microdiffraction mapping: crystal structures from heterogeneous samples, phase distribution and variability  
[Barbara Lavina](#) (Las Vegas/US)
- 11.40-12.00  
IO 28.2 Whitlockite-related  $\text{Ca}_9\text{R}(\text{VO}_4)_7$  (R=La, Nd, Gd) vanadates under high pressure  
[Wojciech Paszkowicz](#) (Warsaw/Poland), K. Kosyl, O. Ermakova, R. Minikayev, J.Z. Domagała, A. Suchocki, D. Włodarczyk, A. Shekhovtsov, M. Kosmyna, C. Popescu, F. Fauth
- 12.00-12.15  
O 28.1 Phase relation of  $\text{MgCO}_3$  high-pressure carbonate under the deep lower mantle conditions  
[Fumiya Maeda](#) (Sendai/Japan), S. Kamada, T. Sakamaki, N. Miyajima, N. Hirao, Y. Ohishi, A. Suzuki
- 12.15-12.30  
O 28.2 A first-principles study and experimental investigation of structural and magnetic properties of  $\text{M1M2}(\text{PO})_4$  olivine-type materials at high-pressure  
[Maribel Núñez-Valdez](#) (Potsdam/Germany), I. Efthimiopoulos, M. Taran, M. Wilke, J. Müller, E. Bykova, M. Koch-Müller
- 12.40-13.00 [Closing Ceremony](#)
- 13.00-14.00 [Lunch](#)



## S 1 – High-pressure chemistry

- P1  
Modification of structure and physical properties of  $\text{MgB}_2$  superconductor due to synthesis under 1 GPa pressure  
Tomasz Cetner (Warsaw/Poland), Andrzej Morawski, Akiyasu Yamamoto, Ryszard Diduszko
- P2  
High-pressure synthesis, structure and equation of state of new tetragonal boron subnitride  $\text{B}_{50}\text{N}_2$   
Kirill Cherednichenko (Villetaneuse/France), Vladimir Solozhenko
- P3  
Topology of the chemical pressure field in simple molecules  
Mikhail Pokryvaylo (Oviedo/Spain), Hussien Osman, Miguel Ángel Salvadó, J. Manuel Recio
- P4  
What can we learn from chemical pressure maps of metals and ionic crystals?  
Alvaro Lobato (Madrid/Spain), Hussien Osman, Miguel Angel Salvado, Mercedes Taravillo Valentin Garcia Baonza, Jose Manuel Recio Muñiz
- P5  
Formation and behavior of metal hydrides at extreme p,T: In situ PXRD studies at ID06-LVP, ESRF  
Kristina Spektor (Grenoble/France), Wilson Crichton, Ulrich Häussermann, Sumit Konar
- P6  
Experimental evidence for stable crystalline polymeric carbon dioxide at lowermost mantle conditions  
Kamil Dziubek (Florence/Italy), Martin Ende, Demetrio Scelta, Roberto Bini, Mohamed Mezouar, Gaston Garbarino, Ronald Miletich
- P7  
Flexible amines – a new route for designing advanced, porous materials  
Aleksandra Półnoliczak (Poznan/Poland), Szymon Sobczak, Andrzej Katrusiak





## S 2 – New phenomena at high pressure

P8  
Metallization of erbium and yttrium trihydrides under high pressure  
Marek Tkacz (Warsaw/Poland), Mikhail Kuzovnikov, Mikhail Eremites, Aleksander Drozdov, Stanislav Besedin

P9  
Pressure-induced conformational conversion in p-tolyl disulfide at phase transition and in a hidden polymorph  
Szymon Sobczak (Poznan/Poland), Andrzej Katrusiak

P10  
Properties of  $\text{YbAu}_2\text{Si}_2$  under hydrostatic pressure  
Jiří Kaštil (Prague/Czech Republic), Kristina Vlášková, Jiří Prchal, Martin Míšek, Jiří Kamarád, Zdeněk Arnold

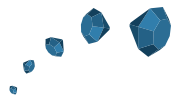
## S 3 – Amorphous materials and liquids under pressure

P11  
Hydrogen content and Raman spectra of amorphous magnesium silicates with Mg/Si from 0 to 0.9 hydrogenated at high pressure  
Vadim Efimchenko (Moscow/Russia), Nikolay Barkovskii, Vladimir Fedotov, Konstantin Meletov, Kirill Khryapin

P12  
Structural evolution of liquid sulphur under pressure  
Gunnar Weck (Bruyères-le-Châtel/France), L. Henry, M. Mezouar, G. Garbarino, F. Datchi

## S 4 – Elements and binary alloys under pressure: structural and electronic transformations

P13  
Raman study of bismuth at high pressure  
Julien Haines (Montpellier/France)



P14

Boron monosulfide: equation of state and pressure-induced phase transition

Kirill Cherednichenko (Villetaneuse/France), Ivan Kruglov, Artem Oganov, Yann Le Godec, Mohamed Mezouar, Vladimir Solozhenko

P15

Pressure induced elimination of ferro-ferro transition in  $\text{Sc}_{0.35}\text{Ti}_{0.65}\text{Fe}_2$  intermetallic compound

Zdenek Arnold (Prague/Czech Republic), Martin Misek, Olivier Isnard, J. Pemeja, Jiri Kastil, Jiri Kamarad

P16

High pressure phase diagram of sulphur from laser-heated diamond anvil cell experiments

Hannah B. Scott (Edinburgh/Great Britain), Tomoaki Kimura, R. Stewart McWilliams

#### S 5 – Materials chemistry at high pressure

P17

Synthesis by sol gel route, structural and dielectric characterization of cerium doped lead zirconium titanate

El Miloudi El Moussafir (Casablanca/Maroko)

P18

Phosphorus doping in (111) face of single crystal diamond grown by the temperature gradient HPHT method

Sergei Buga (Moscow/Russia), Vitaly Bormashov, Jullien Bargon, Michail Kuznetsov, Sergei Terentiev, Sergei Tarelkin, S Temgoua, Vladimir Blank

P19

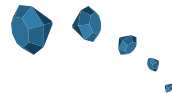
Post-spinel transition in hausmannite determined by high P-T in situ X-ray diffraction

Jolanta Darul (Poznan, Poland), Christian Lathe, Pawel Piszora

P20

Crystal packing diversity of the simple amidinate oxozinc complex derived by non-covalent interactions

Michał Terlecki (Warsaw/Poland), Michał Leszczyński, Szymon Sobczak, Iwona Justyniak, Andrzej Katrusiak, Janusz Lewiński



P21

Dimerization in the III-V semiconductor gallium phosphide

Barbara Lavina (Las Vegas, USA)

P22

High pressure magnetic characterisation of the elpasolite  $\text{La}_2\text{NiMnO}_6$   
Christopher Ridley (Didcot/Great Britain), Nicholas Funnell, Craig Bull

P23

Pressure-induced broadening of photoluminescence from Bismuth-doped glasses  
John Proctor (Salford/Great Britain), Robert McMaster, Malik Hakeem, Mark Hughes

### S 6 – Superconductivity under high pressure: Experiment and theory

P24

Development of a symmetric miniature diamond anvil cell for magnetic measurements in a SQUID magnetometer and structural studies

Bastien Guigue (Paris/France)

P25

Pressure – induced metallization and superconductivity in the transition metal dichalcogenides  $\text{MX}_2$

Moaz ElGhazali (Dresden/Germany)

P26

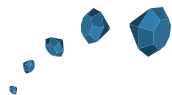
Strong electron-phonon and band structure effects in the optical properties of superconducting hydrogen

Miguel Borinaga (Donostia-San Sebastian/Spain), Julen Ibañez-Azpiroz, Aitor Bergara, Ion Errea

P27

Formation process of high- $T_c$  phase of sulfur hydride

Mari Einaga (Toyonaka, Japan), Masafumi Sakata, Akiyoshi Masuda, Harushige Nakao, Katsuya Shimizu, Alexander Drozdev, Mikhail Eremets, Saori Kwaguchi, Naohisa Hirao, Yasuo Ohishi



### S 7 – Critical and supercritical fluids under pressure

P28

High pressure processing for the pharmaceutical compounds using the supercritical fluid technology

Yan-Ping Chen (Taipei/Taiwan), Chun-Hao Fang, Chun-Ta Chen, Muoi Tang, Sheau-Ling Ho

P29

High pressure synthesis of a temperature and pH-sensitive copolymer using the supercritical fluid technology

Muoi Tang (Taipei/Taiwan), Sheau-Ling Ho, Yan-Ping Chen

### S 8 – High pressure structural analysis and (meta)data deposition

P30

DAC-XRD: Data management and processing framework for high-pressure X-ray diffraction experiments with diamond anvil cells

Anna Makal (Warsaw/Poland), Jaroslaw Kalinowski

P31

Synthesis, characterization, crystal structure determination and theoretical study of some new rhenium(I)-tricarbonyl complexes with 2,2'-bipyridine and 2,9-dimethylphenanthroline ligands

Fatemeh Safari (Tehran,Iran)

### S 9 – High-pressure instrumentation

P32

Electric discharge machine for drilling diamond anvil cell gasket holes

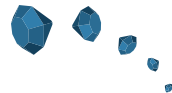
John Proctor (Salford/Great Britain), Daniel Massey, Stuart Astin

### S 10 – New techniques at large scale facilities

P33

Melting dynamics of water ices in the mesoscopic regime

Naomi Falsini (Florence/Italy), Margherita Citroni, Samuele Fanetti, Paolo Foggi, Roberto Bini



### S 11 – Porous framework under pressure

P34

Three polymorphous crystals with large channel network studied by SXRD

Tamás Holczbauer (Budapest/Hungary), Dániel Vajk Horváth, Petra Bombicz, Tibor Soós

### S 12 – High pressure crystallographic studies

P35

High-pressure study of the crystal structure of disodium 2-amino-6-oxo-6,7-dihydro-1H-purine-1,7-diide heptahydrate

Anna Gaydamaka (Novosibirsk, Russia), Sergey Arkhipov, Boris Zakharov, Yuriy Seryotkin, Elena Boldyreva

P36

Compressed interactions and properties of methylamines

Marcin Podsiadło (Poznan/Poland), Anna Olejniczak, Andrzej Katrusiak

P37

Pressure dependence of an unusual structural transition in a molecular Spin-CrossOver compound revealed by Powder X-ray Diffraction under pressure

Elodie Tailleur (Bordeaux/France), Mathieu Marchivie, Jean-Paul Itie, Philippe Guionneau

P38

High-pressure structures of meta-dichlorobenzene and dibromobenzene

Karolina Kwaśna (Poznan/Poland), Michalina Anioła, Weizhao Cai, Andrzej Katrusiak

P39

High-pressure preference for the low Z' polymorph of a molecular crystal

Kinga Roszak (Poznan/Poland), Anna Katrusiak, Andrzej Katrusiak

P40

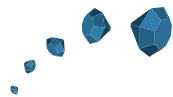
Giant anomalous strain between high-pressure phases and the mesomers of urea

Kinga Roszak (Poznan/Poland), Andrzej Katrusiak

P41

Pressure effect on the complication of crystal structures the case study on 6-chloro-4,4,5,7-tetramethyldihydrocoumarin

Ida Bukalska (Poznan/Poland), Kacper Rajewski, Andrzej Katrusiak



## Poster presentations • Monday, 4 September & Thursday, 7 September 2017

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P42

High-pressure polymorphism of 4,4'-bipyridine perchlorate

Michalina Anioła (Poznan/Poland), Andrzej Katrusiak

P43

Disappearing polymorphs of 2,4,5-triiodoimidazole

Kacper Wojciech Rajewski (Poznan/Poland), Michał Andrzejewski, Andrzej Katrusiak

P44

High pressure studies of 4,5 – dichloroimidazole

Karolina Fercz (Poznan/Poland), Kacper Rajewski, Andrzej Katrusiak

P45

Solvent-effect for the stability and compression of a noncovalent porous material WUT-Ni

Karolina Fercz (Poznan/Poland), Kacper Rajewski, Katarzyna Sołtys, Andrzej Katrusiak

P46

Pressure effect on the arene-perfluoroarene interaction

Alexandra Friedrich (Wuerzburg/Germany), Krzysztof Radacki, Javier Ruiz-Fuertes, Ines E. Collings, Daniel Sieh, Todd B. Marder

P47

Halogen and hydrogen bonds in compressed pentachloroethane

Marcin Podsiadło (Poznan/Poland), Maciej Bujak, Andrzej Katrusiak

P48

High pressure behavior of  $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{Br}_2$  as a member of photosalient cobalt(III)

Boris Zakharov (Novosibirsk/Russia), A.S. Marchuk, Elena Boldyreva

### S 13 – Synchrotrons and neutron high-pressure facilities

P49

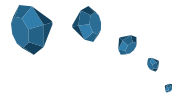
Opportunities for high-pressure science at the European Spallation Source

Malcolm Guthrie (Lund/Sweden), Arno Hiess

P50

Towards resonant X-ray scattering at high pressure: strategy and first results

Isabel Povedano (Edinburgh/Great Britain), Daniel Porter, Konstantin Kamenev, Alessandro Bombardi



S 14 – Pressure induced quantum criticality and novel emergent phases

P51

Magnetism of  $U_4Ru_7Ge_6$  under high pressures

Martin Míšek (Prague/Czech Republic), Jan Prokleška, Michal Vališka, Petr Proschek, Jaroslav Valenta, Jiří Kaštil, Jiří Kamarád, Martin Diviš, Vladimír Sechovský

S 15 – High-pressure spectroscopy and structural studies of new materials

P52

Aniline-derived arrays polymerized at high-pressure and high-temperature

Marcelo Nobrega (São Paulo/Brazil), Erico Teixeira-Neto, Andrew Cairns, Marcia Temperini, Roberto Bini

P53

High-pressure structural and optical properties of organometal halide perovskites

Kai Wang (Changchun/China)

P54

Unusual structural transition in  $CaCo_3V_4O_{12}$  double perovskite under high pressure

Sergey Ovsyannikov (Bayreuth/Germany)

P55

High-pressure phase of scintillating cadmium tungstate

Daniel Errandonea (Valencia/Spain) Javier Ruiz-Fuertes, A. Friedrich, A. Segura, W. Morgenroth, P. Rodriguez-Hernandez, A. Muñoz, Y. Meng

P56

Stability of the benzene molecule to above 50 GPa at 300 K

John Proctor (Salford/Great Britain), Saba Shaikh, Francis Barber, Malik Hakeem

P57

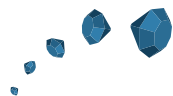
Kevlar® fibres under hydrostatic pressure by means of Raman spectroscopy

Dimitris Christofilos (Thessaloniki/Greece)

P58

High pressure Raman and photoluminescence studies of  $In_xAl_{1-x}N$  alloys

Dimitris Christofilos (Thessaloniki/Greece)



P59

The possibility of new multiple calcium polyhydride structural phases synthesized under high pressure and high temperature

Takaki Muramatsu (Bristol/Great Britain), Muhtar Ahart, Maddury Somayazulu, Russell Hemley

P60

Ab initio theoretical study of rare-earth orthophosphates  $APO_4$  (with A=La, Sc, and Y) under pressure

Andres Mujica (La Laguna/Spain), Silvana Radescu, Javier Lopez-Solano, Placida Rodríguez-Hernandez, Alfonso Muñoz

### S 16 – Theoretical prediction of high-pressure phases

P61

Dynamical and elastic properties of  $MgSO_4$  under high pressure from ab initio simulations

Alejandro Jorge-Montero (La Laguna/Spain), Plácida Rodríguez-Hernández, Alfonso Muñoz

P62

Structural and electronic properties of  $WX_2$  dichalcogenides at high pressure

Oto Kohulák (Bratislava/Slovakia), Roman Martoňák

P63

Structural evolution of amorphous polymeric nitrogen from ab initio simulations

Dominika Vlčková (Bratislava/Slovakia), Oto Kohulák, Dušan Plašienka, Roman Martoňák

### S 17 – Shock experiments and ultra-high pressure generation

P64

Diffraction studies of phase transitions and strength in vanadium

Michael Stevenson (Edinburgh/Great Britain)

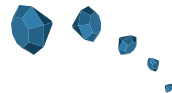
### S 18 – High-pressure life and biosciences

P65

A radiant GRIN at high pressure: Utilizing gradient index lenses to enable multiphoton microscopy at hydrostatic pressure up to 200 MPa

Dominik Schneider (Erlangen/Germany)





P66

Comparative study of structural and activity changes of HIV-1 protease and its covalently linked dimer under high pressure

Marek Ingr (Zlín/Czech Republic), Laetitia Palmade, Tařána Majerová, Dominique Chevalier-Lucia, Eva Kutáľková, Josef Hrnčičík, Reinhard Lange

P67

Macromolecular crowding and pressure: crowding agents destabilize proteins in low concentration, but stabilize them in high concentration against pressure unfolding

László Smeller (Budapest/Hungary), Zsofia Török, Frederik Pfalzgraf, Judit Somkuti

### S 20 – High-pressure studies in the Earth & planetary sciences

P68

Ab initio study of the high pressure phase of the CO<sub>2</sub> clathrate hydrate

J. Manuel Recio (Oviedo/Spain), Fernando Izquierdo-Ruiz, Olga Prieto-Ballesteros

P69

Spectroscopic properties of natural jarosite under high pressure

Alvaro Lobato (Madrid/Spain), Miriam Peña-Alvarez, Ana Isabel Casado, Valentin Garcia Baonza, Mercedes Taravillo

P70

Single crystal x-ray diffraction of forsterite III to 160 GPa

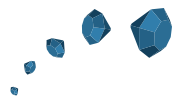
Barbara Lavina (Las Veegas/USA), Sally Lee, Minta C Akin, Paul D Asimow, M. Homel, RS Crum, D Pagan, J Lind, Joel V bernier, JL Mosenfelder, AM Dillman, OV Fat'Yanov, MG Newman

### S 22 – Food science and technology

P71

Potential of high pressure technology to inactivation of *Lactobacillus brevis* in beer

Justyna Nasiłowska (Warsaw/Poland), Barbara Sokołowska, Marzena Woszczyk, Dorota Michałowska, Adrianna Raczkowska



P72

Optimization of high hydrostatic pressure extraction by response surface methodology of bioactive compounds from stinging nettle

Jorge Saraiva (Aveiro/Portugal), Silvia Moreira, Elisabete Alexandre, Manuela Pintado

P73

Brewing characteristics of piezosensitive Sake – yeasts

Kazuki Nomura (Niigata/Japan), Hirofumi Hoshino, Kazuaki Igoshi, Haruka Onozuka, Mayumi Hayashi, Harutake Yamazaki, Hiroaki Takaku, Akinori Iguchi, Toru Shigematsu

P74

A pilot study of combinations of ultrasonication pre-treatment and high pressure processing effecting microbial inactivation and rheological attributes of liquid egg yolk

Adrienn Tóth (Budapest/Hungary), Csaba Németh, Rebeka Csáti, Réka Juhász, Barbara Csehi, László Friedrich

P75

High pressure processing of baby foods: inactivation of *saccharomyces cerevisiae* and evaluation of sensory attributes in fruits base product for babies and infants during long shelflife

Bożena Mazurkiewicz (Warsaw/Poland)

### S 23 – Energy materials under high pressure: experiment and theory

P76

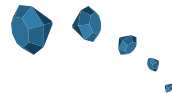
Combined theoretical and experimental investigations of pressure-driven phase transition in  $\text{InNbO}_4$

Alfonso Muñoz (La Laguna/Spain), Placida Rodríguez-Hernandez, Daniel Errandonea, Alka B Garg, Catalin Popescu, Domingo Martinez-Garcia, Juan A Sans, Vanesa Cuenca-Gotor, Pablo Botella

P77

Structural and vibrational study of monoclinic  $\text{As}_2\text{S}_3$  at high pressure

Vanesa Paula Cuenca-Gotor (València/Spain), Juan Ángel Sans, Francisco Javier Manjón, Catalin Popescu, Silvana Radescu, Andrés Mujica, Plácida Rodríguez-Hernández, Alfonso Muñoz, Jordi Ibáñez



P78

The effect of pressure on hydrogen solubility in Zircaloy nuclear fuel cladding

John Proctor (Salford/Great Britain), Hannah Weekes, Dean Smith, Cristina Simionescu, Timothy Prior, Mark Wenman, David Dye

P79

High-pressure studies of high-nitrogen-content 6-azido-1,2,3,4-tetrazolo-[1,5-b]-pyridazine

Anna Olejniczak (Poznan/Poland), Anna Katrusiak, Andrzej Katrusiak

P80

Vibrational study of  $\text{In}_2\text{Se}_3$  under high pressure

Rosario Vilaplana (València/Spain), Samuel Gallego, Alfonso Muñoz, Plácida Rodríguez-Hernández, Francisco Javier Manjón, Alfredo Segura, Daniel Errandonea

P81

Effect of pressure on  $\text{Li}_{0.5}\text{Ni}_{0.5}\text{Mn}_2\text{O}_4$ : New quaternary mixed metal oxide – bridging the gap between  $\text{LiMn}_2\text{O}_4$  and  $\text{NiMn}_2\text{O}_4$

Paweł Piszora (Poznań/Poland), Jolanta Darul, Dörthe Haase

## S 24 – Physics and transformations in compressed matter

P82

A modified system for low temperature experiments in a 3000 ton multi-anvil press

Rick Secco (London/Canada), Wenjun Yong

## S 26 – Novel magnetic-electronic behavior at extreme P-T

P83

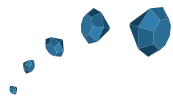
Pressure effect on metamagnetic transition in  $\text{UIrSi}_3$

Jaroslav Valenta (Prague/Czech Republic), Fuminori Honda, Jiří Kaštil, Jiří Prchal, Vladimír Sechovský

P84

High-pressure effect on magnetism and valence of  $\text{YbPd}_2\text{Si}_2$

Jiří Prchal (Prague/Czech Republic), Jan Fikáček, Jan Prokleška, Jiří Kaštil, Kristina Vlášková, Marie Kratochvílová, Martin Diviš



### S 27 – Structural phase transitions theory and experiment

P85

Bonding indicators for the analysis of pressure-induced structural phase transitions  
Olga Matthies (Dresden/Germany), Yuri Grin, Miroslav Kohout

### S 28 – High pressure mineral physics and geochemistry

P86

Densification of calcium-aluminum-silicate glass at the pressure of ~5.5 GPa  
Ayano Nakajima (Sendai/Japan), Tatsuya Sakamaki, Naoki Hisano, Yoshiki Horioka,  
Tomonori Ohashi, Akio Suzuki

P87

Electrical resistivity of Fe, Co and Ni along their melting boundaries  
Rick Secco (London/Canada), Reynold Silber, Innocent Ezenwa, Wenjun Yong, Joshua  
Littleton

P88

Thermodynamic properties of (Mg,Fe)-silicates at mantle conditions and geophysical  
implications  
Tatiana Sokolova (Irkutsk/Russia), Peter Dorogokupets

P89

High pressure behaviour of kalsilite-O1  
Clivia Hejny (Innsbruck/Austria), Biljana Krüger

P90

X-ray diffraction study of rhodium oxyhydroxide at high pressure  
Akio Suzuki (Sendai/Japan), Yoshiki Horioka, Naoki Hisano

P91

Decomposition of fayalite at high hydrogen pressure  
Vadim Efimchenko (Moscow/Russia), Nikolay Barkovskii, Vladimir Fedotov, Konstantin  
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---

A

Ahuja 8, 9, 53, 54, 58, 68, 92,  
Alabarse 54, 66, 92,  
Andrzejewski 24, 69, 85,  
Aniola 54, 64, 84, 85, 92,  
Aprilis 54, 72, 92,  
Arnold 80, 81, 92,

B

Barbour 54, 64, 65, 92,  
Biswas 55, 77, 92,  
Boehler 54, 64, 66, 72, 92,  
Boldyreva 1, 6, 41, 42, 43, 55, 75, 84,  
85, 92,  
Botella 55, 74, 89, 92,  
Botella Vives 55, 74, 92,  
Braun 54, 64, 92,  
Brooks 8, 54, 71, 92,  
Buga 8, 9, 81, 92,  
Bukalska 84, 92,  
Bull 54, 61, 65, 66, 74, 82, 92,

C

Cao 53, 57, 60, 61, 93,  
Capitani 53, 59, 93,  
Casati 54, 62, 65, 93,  
Castillo 57,  
Ceppatelli 53, 56, 60, 74, 93,  
Cetner 79, 93,  
Chen 83, 93,  
Cherednichenko 79, 81, 93,  
Coleman 54, 70, 93,  
Contreras-García 67, 75,  
Cuenca-Gotor 75, 89, 93,  
Cywinski 77,

D

Darul 10, 81, 90, 93,  
Degtyareva 9  
Dera 1, 6, 44, 45, 46, 47, 55, 74, 76, 93,  
Ding 55, 74, 93,  
Drozd 61,  
Dubrovinskaia 1, 6, 8, 9, 24, 36, 37, 53,  
54, 60, 63, 69, 72, 93  
Dubrovinsky 1, 6, 24, 48, 49, 53, 54, 56,  
63, 65, 69, 70, 72, 76, 93,  
Dziubek 53, 56, 60, 61, 65, 74, 79, 93,

E

Efimchenko 80, 91, 94,  
ElGhazali 58, 82,  
El Moussafir 81, 94,  
Errandonea 54, 56, 68, 86, 89, 90, 94,  
Errea 55, 77, 82, 94,

F

Fabbiani 9, 54, 65,  
Falsini 57, 83, 94,  
Fercz 85, 94,  
Fidalgo 55, 73, 94,  
Friedrich 8, 9, 68, 85, 86, 89, 94, 101,  
Friese 9  
Fuchizaki 53, 58, 94,  
Funnell 54, 65, 66, 74, 82, 94,

G

Gabarino 8  
Garbarino 53, 54, 57, 58, 59, 63, 66, 68,  
79, 80, 94,  
Gawraczyński 55, 56, 60, 75, 94,  
Gaydamaka 84, 94,  
Gładysiak 65,  
Gomez-Perez 64,



## Participants list

---

Gonzalez 9  
Gorelli 8, 9, 74  
Graf 54, 63, 95,  
Grochala 53, 56, 60, 69, 75, 95,  
Grzegory 9, 53, 60, 61,  
Grzelak 53, 56, 60, 75, 95,  
Guigue 82, 95,  
Guńka 54, 65, 95,  
Guthrie 54, 56, 64, 66, 72, 74, 85, 95,

### H

Haase 54, 67, 90, 95,  
Haberl 54, 64, 66, 72, 95,  
Haines 9, 53, 54, 60, 66, 74, 80, 95,  
Hakeem 54, 61, 68, 82, 86, 95,  
Hanfland 53, 59, 65, 95,  
Hartley 54, 70, 71, 95,  
Hase 58,  
Hearne 9, 55, 76, 95,  
Heiny 9  
Hejny 54, 65, 91, 95,  
Hernandez 8, 86, 87, 89  
Holczbauer 84, 95,  
Huxley 77,

### I

Ingr 88, 95,

### J

Jaroń 56, 60, 75,  
Jin 53, 58,  
Jorge-Montero 87,  
Jurczak 9

### K

Kalbitzer 54, 71, 96,

Kamenev 8, 9, 54, 57, 63, 77, 85,  
Kaminska 54, 67, 96,  
Kaštil 80, 86, 90, 96,  
Katrusiak 7, 9, 10, 11, 44, 57, 64, 65, 79,  
80, 81, 84, 85, 90,  
Kepa 55, 77, 96,  
Khasanov 54, 63,  
Khomskii 55, 76, 96,  
Kim 55, 75, 96,  
Klotz 8, 9, 53, 54, 57, 66, 96,  
Knap 55, 67, 77, 96,  
Kohulák 87, 96,  
Kralj 53, 61, 96,  
Kraus 54, 70, 71, 96,  
Krukowski 67,  
Kumar 59,  
Kurzydłowski 54, 56, 60, 69, 75, 96,  
Kvashnin 54, 69, 96,  
Kwaśna 84, 96

### L

Laniel 53, 60, 97,  
Lavina 54, 55, 72, 78, 82, 88, 97,  
Lazarev 54, 71, 97,  
Lazicki 71  
Lee 55, 70, 74, 75, 77, 88, 97,  
Leszczyński 56, 60, 75, 81,  
Li 53, 54, 57, 60, 61, 64, 97,  
Liu 9, 58, 60, 61, 66, 71,  
Loa 8, 9, 53, 59, 77, 97,  
Lobato 79, 88, 97,

### M

Machon 8  
Maeda 55, 72, 78, 97,  
Makal 83, 97,  
Makohonienko 1, 6, 50, 51, 52, 55, 73,

Malinowska-Pańczyk 73, 97,  
Mañosa 53, 57,  
Mao 1, 6, 33, 34, 35, 53, 56, 97  
Marchivie 53, 62, 68, 84, 97,  
Marqués 53, 59, 67,  
Martinez-Canales 55, 77, 97,  
Martinez-Garcia 56, 89,  
Martoňák 54, 55, 68, 77, 87,  
Matthies 54, 67, 91, 98,  
Mazurkiewicz 89, 98,  
McMonagle 54, 63, 64, 98,  
McWilliams 54, 64, 70, 81, 98,  
Medvedev 53, 58, 59, 98,  
Meersman 8, 9  
Meier 55, 57, 76, 98,  
Meng 47, 53, 57, 60, 61, 74, 86, 98,  
Meyer 53, 62, 98,  
Mezouar 9, 58, 59, 60, 65, 66, 79, 80, 81  
Michiels 1, 6, 38, 39, 40, 54, 70, 98,  
Miguel 9, 77, 79, 82, 92, 97  
Míšek 80, 86, 98,  
Moggach 54, 63, 64, 98,  
Monteseguro-Padrón 68,  
Montisci 53, 62, 98,  
Mujica 87, 89, 98,  
Munoz 89, 98,  
Muñoz 67, 68, 75, 86, 87, 89, 90,  
Muramatsu 87, 98,

## N

Nakajima 91, 98,  
Nasiłowska 55, 73, 88, 99,  
Nobrega 86, 99,  
Nomura 89, 99,  
Núñez-Valdez 55, 78,

## O

Oganov 69, 81,

Ohira 54, 72, 99,  
Olejniczak 10, 84, 90, 99,  
Orlikowski 54, 64, 99,  
Ovsyannikov 55, 76, 86, 99,

## P

Pakhomova 54, 65, 66, 72, 99,  
Paliwoda 53, 58, 99,  
Pashkin 64,  
Pasternak 8, 9, 76,  
Paszkwicz 55, 78, 99,  
Paz-Pasternak 8, 9  
Peña-Álvarez 53, 57,  
Pépin 53, 60, 99,  
Pinkowicz 53, 55, 57, 76, 99,  
Piotrowicz 10  
Piszora 7, 10, 81, 90, 99,  
Plisson 54, 58, 63, 99,  
Podsiadło 8, 10, 84, 85, 99,  
Pokryvaylo 79, 100,  
Pórolniczak 79, 100,  
Povedano 85, 100,  
Prchal 8, 9, 80, 90, 100,  
Proctor 53, 61, 68, 82, 83, 86, 90, 100,  
Pruteanu 53, 58, 100,  
Pulham 55, 74, 75,

## Q

Qi 53, 55, 57, 59, 74, 100,

## R

Rajewski 84, 85, 100,  
Ratajczak-Sitarz 10  
Recio 8, 9, 79, 88, 100  
Redfern 55, 76, 77,  
Ridley 55, 65, 66, 74, 77, 82, 100,  
Rietveld 54, 71, 100,



## Participants list

---

Rodríguez 8, 67, 68, 75, 87, 89, 90,  
Rodríguez-Hernández 67, 68, 75, 87, 89, 90,  
Rosa 54, 62, 68, 100,  
Roszak 84, 100,  
Rozenberg 55, 76,  
Rzoska 53, 55, 61, 73, 100,

### S

Sadovyi 53, 60, 100,  
Safari 83, 100,  
Sans 55, 67, 68, 75, 89, 100,  
Santamaría-Pérez 53, 56, 61,  
Santoro 55, 74, 101,  
Saraiva 8, 9, 55, 73, 89, 101,  
Saxena 54, 66,  
Scandolo 8, 9, 54, 55, 69, 77, 101,  
Scelta 53, 56, 60, 74, 79, 101,  
Schneidereit 87, 101,  
Schwarz 53, 57, 59, 101,  
Scott 64, 81, 101,  
Secco 90, 91, 101,  
Shakhov 54, 71, 101,  
Smeller 9, 54, 70, 71, 88, 101,  
Śmiechowski 53, 61, 102,  
Sobczak 24, 54, 64, 69, 79, 80, 81, 101,  
Sokolova 91, 101,  
Sokołowska 73, 88,  
Spektor 79, 101,  
Spiekermann 54, 68, 101,  
Stekiel 54, 72, 101,  
Stevenson 70, 87, 101,  
Struzhkin 56, 60, 75,  
Suzuki 72, 78, 91, 101,

Svitlyk 53, 59, 60, 66, 102,  
Szafranski 53, 57,

### T

Tailleur 62, 84, 102,  
Tang 83, 102,  
Taravillo Corralo 53, 56,  
Tateiwa 54, 67, 102,  
Terlecki 81, 102,  
Tkacz 9, 55, 74, 80, 102,  
Tóth 89, 102,  
Tulk 54, 56, 66, 72, 102,

### V

Valenta 86, 90, 102,  
Vlčková 87, 102,  
Vondracek 53, 60, 102,

### W

Wang 54, 60, 61, 67, 71, 75, 86, 102,  
Weck 53, 54, 57, 58, 60, 64, 80, 102,  
Wesołowska 55, 73, 102,

### Y

Yahniuk 54, 67, 77, 103,

### Z

Zakharov 53, 54, 61, 65, 84, 85, 103,  
Zhang 54, 55, 71, 73, 77, 103,  
Zimmer 53, 61, 103,



Notes

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## Notes

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