

Joint Meeting

Deutsche Gesellschaft für Kristallographie (DGK)
German Crystallographic Society
(19th Annual Meeting)



Deutsche Mineralogische Gesellschaft (DMG)
German Mineralogical Society
(89th Annual Meeting)



Österreichische Mineralogische Gesellschaft (ÖMG)
Austrian Mineralogical Society
(MinPet 2011)



Crystals, Minerals and Materials

20–24 September 2011 • Salzburg, Austria



PROGRAMME

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Organisation and Imprint

Venue

University of Salzburg
Faculty of Natural Science
Hellbrunnerstraße 34* • 5020 Salzburg (Austria)

Scientific Organisation

German Crystallographic Society (DGK)
German Mineralogical Society (DMG)
Austrian Mineralogical Society (ÖMG)

Conference Chair

O. Univ.-Prof. Dr. Georg Amthauer
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Local Organising Committee

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Conference Organisation

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Conference Website

www.salzburg2011.org

Design/Layout

Layout	www.krea.tif-design.de
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Circulation	500
Editorial Deadline	26 July 2011

*please find detailed information for arriving the venue at page 62

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Welcome Notes

Dear Colleagues,

It is a great pleasure for the organising committee to invite you to the upcoming Joint Meeting of the German Crystallographic Society, the German Mineralogical Society, and the Austrian Mineralogical Society. You are cordially invited to attend the conference which will be held at the University of Salzburg, Faculty of Natural Sciences, 20–24 September, 2011. Scientific sessions as well as plenary lectures on different topics of current interest will cover a wide range of fields from mineral resources to high-tech materials to protein crystallography and will show the unique position of crystallography and mineralogy between physics, chemistry, biology, and material sciences. We are looking forward to your attendance and contributions from all fields of crystallographic and mineralogical research.

With kind regards
On behalf of the organising committee



O. Univ.-Prof. Dr. Georg Amthauer
Conference Chair

Liebe Kolleginnen und Kollegen,

als Präsident der Österreichischen Mineralogischen Gesellschaft (ÖMG) ist es mir eine besondere Freude, Sie im Namen unserer Vereinigung in diesem Jahr in Salzburg begrüßen zu können. Länderübergreifende mineralogisch-kristallographische Tagungen haben im deutsch-österreichischen Raum ja schon durchaus eine gewisse Tradition. Es sei an dieser Stelle an die DMG-ÖMG-Gemeinschaftstagung in Salzburg im Jahr 1991, an die 1999 in Wien abgehaltene Gemeinschaftstagung der Deutschen Mineralogischen Gesellschaft und der ÖMG sowie an das im Jahr 2005 in Köln von der Deutschen Gesellschaft für Kristallographie, der Deutschen Gesellschaft für Kristallwachstum und Kristallzüchtung sowie dem Nationalkomitee für Kristallographie der Österreichischen Akademie der Wissenschaften veranstaltete Meeting erinnert. Sowohl im Titel „Crystals, Minerals and Materials“ als auch in dem von den Organisatoren zusammengestellten Programm wird der fächerübergreifende Charakter dieses Treffens betont. Ich persönlich halte diesen interdisziplinären Aspekt für eine wirkliche Chance, einmal über den eigenen „fachlichen Tellerrand“ hinauszublicken. Gerade im Bereich der Mineralogie haben wir in letzten Jahren eine zunehmend strikte Separierung in erdwissenschaftliche und materialwissenschaftliche Arbeitsrichtungen erlebt, eine Entwicklung, die unserer Disziplin nicht immer zum Vorteil gedient hat. In diesem Sinn wünsche ich der Tagung einen guten Verlauf und allen Teilnehmern und Teilnehmerinnen viel Erfolg bei der Präsentation und im wissenschaftlichen Diskurs der aktuellen Forschungsergebnisse.

Ihr



Volker Kahlenberg
Präsident der ÖMG

Programme Overview • Tuesday, 20 September 2011

	HS 401	HS 434	HS 414	HS 421	
08:30					
09:00					
10:00					
11:00					
12:00					
13:00					
14:00	Registration		DMG Board Meeting	DGK Board Meeting	
15:00			p. 15	p. 15	
16:00	Opening				
17:00	Break				
17:15	Awards				
18:00					
19:00	p. 15				
19:15	Get-Together				
20:00					p. 59

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- Solicit new members

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Programme Overview • Wednesday, 21 September 2011

	HS 401	HS 402	HS 403	HS 434
08:00	Registration			
08:15				
08:30				
09:00	G. Dehm			
09:15				
09:30				
09:45		p. 16		
10:00	Coffee Break			
10:15				
10:30	MS 1	MS 2	MS 3	MS 4
10:45	Crystallography	Functional Materials I	Metamorphic and	Computational
11:00	at High Pressure/ Temperature		Magmatic Processes I	Crystallography
11:15				
11:30				
11:45				
12:00				
12:15	p. 16	p. 17	p. 18	p. 19
12:30				
12:45	Lunch Break	Lunch Symposium	Lunch Break	
13:00		Bruker AXS		
13:15				
13:30		p. 19		
13:45				
14:00	J.D. Clemens			
14:15				
14:30				
14:45	p. 19			
15:00	Poster Presentation and Coffee Break			
15:15				
15:30				
15:45				
16:00	MS 5	MS 6	MS 7	MS 8
16:15	Synchrotron- and	Functional	Metamorphic and	Archeomaterials
16:30	Neutron Diffraction	Materials II	Magmatic Processes II	p. 23
16:45		and Ionic Conductors	and Thermodynamics	Break
17:00			p. 22	MS 10
17:15			MS 9	Mineralogy at School
17:30			Thermodynamics and	
17:45	p. 20	p. 21	Energetics of Earth	p. 24
17:55			Materials p. 23	
18:00				
18:15				
18:30				
18:45				
19:00	DGK Members Meeting			
19:15				
19:30				
19:45				
20:00	J.G. Bednorz			
20:15				
20:30	p. 24			

Programme Overview • Thursday, 22 September 2011

	HS 401	HS 402	HS 403	HS 434
08:00	Registration			
08:15				
08:30				
09:00	P. Whitfield			
09:15				
09:30				
09:45	p. 25			
10:00	Coffee Break			
10:15				
10:30	MS 11	MS 12	MS 13	MS 14
10:45	Inorganic Structures I	Functional Materials III (CSH-Phases and Phosphates)	Mineral Resources for High-Tech Materials	Bio-Crystallography I
11:00				
11:15				
11:30				
11:45				
12:00				
12:15	p. 25	p. 26	p. 27	p. 28
12:30				
12:45	Lunch Break	Lunch Symposium FEI Company	Lunch Break	
13:00				
13:15				
13:30		p. 28		
13:45				
14:00	E. Conti			
14:15				
14:30				
14:45	p. 28			
15:00	Poster Presentation and Coffee Break			
15:15				
15:30				
15:45				
16:00	MS 15	MS 12	MS 16	MS 17
16:15	Inorganic Structures II	Functional Materials III p. 30	New Methods in Analyses of Mineral Resources p. 30	Bio-Crystallography II
16:30				
16:45		Break		
17:00		MS 18	MS 19	
17:15		Mineral- and Crystal Surfaces	Environmental Mineralogy and Geochemistry I	
17:30				
17:45	p. 29		p. 33	
18:00		p. 32		p. 31
18:15	DMG Members Meeting			
18:30				
18:45				
19:00				
19:15				
19:30	p. 33			
19:45				
20:00	Social Evening			
23:30				p. 60

Programme Overview • Friday, 23 September 2011

	HS 401	HS 402	HS 403
08:00	Registration		
08:30			
09:00	K. Bente		
09:30	p. 34		
10:00	F.M. Meyer		
10:30	p. 34		
11:00	Farewell and Outlook 2012 p. 34		
11:15	Coffee Break		
11:30	MS 20 Environmental Mineralogy and Geochemistry II	MS 21 Spectroscopy of Minerals	MS 22 Molecular Chemistry
12:00			
12:30			
12:45		p. 35	
13:00	p. 34		p.36
20:00	Orchestra concert		
22:00	p. 61		

19 and 20 September 2011

09⁰⁰–17⁰⁰ **Calorimetry in the Geosciences – theory, experiment and applications**

HS 434

Convener E. Dachs, C.A. Geiger, A. Benisek (Salzburg/AT)

A two-day workshop on “Calorimetry in the Geosciences” will be held prior to the start of the DMG-ÖMG-DGK Meeting in Salzburg, Austria in September 2011. The plan of topics and lectures is as follows:

Theory: Basic thermodynamic concepts (C.A. Geiger/E. Dachs)
 Lattice dynamics (E. Dachs/M. Grodzicki)
 Phase diagrams (C.A. Geiger)

Experiment: Low-temperature Calorimetry (E. Dachs)
 Differential Scanning Calorimetry (A. Benisek)
 Solution Calorimetry (J. Majzlan/K. Grevel)

Applications: Calorimetry and activity models – Feldspars (A. Benisek)
 Calorimetry and internally consistent thermodynamic data sets (K. Grevel)
 Calorimetry and garnet solid solutions (C.A. Geiger)

The workshop will take place on 19 and 20 September, 2011 from 9⁰⁰–17⁰⁰ in the “Fachbereich für Materialforschung & Physik” at Salzburg University.

The cost is 50 EUR for regular participants and Ph.D. candidates and is free for M.S. students and undergraduates.

The workshop is included into the list of DMG short courses and workshops. DMG student members will be supported with 50 EUR for travel expenses by application.

A minimum of 10 participants will be needed to give the workshop.

For further details and registration contact: Edgar Dachs, edgar.dachs@sbg.ac.at

Workshops

Monday, 19 September 2011

09⁰⁰–17⁰⁰ **Neutronenstreuung für Kristallographen I**
C 3006
Convener M. Meven (Munich/DE), G. Redhammer (Salzburg/AT)

09⁰⁰ Begrüßung
09¹⁵ Pulvermethoden – Kristallstruktur
10⁰⁰ Pulvermethoden – Magnetismus
10⁴⁵ Kaffeepause
11¹⁵ Einkristalldiffraktion – Kristallstruktur
12⁰⁰ Einkristalldiffraktion – Magnetismus
12⁴⁵ Mittagspause
14⁰⁰ Spektroskopie – Phononen und Magnonen
14⁴⁵ Diffuse Streuung
15³⁰ Kaffeepause
16⁰⁰ Materialwissenschaften
16⁴⁵ Weiche Materie

Tuesday, 20 September 2011

08³⁰–15⁰⁰ **Neutronenstreuung für Kristallographen II**
 Besichtigung FRM II/Garching

08³⁰ Abfahrt Salzburg – FRM II/Garching
10³⁰ Führung durch den FRM II
13⁰⁰ Mittagspause
14⁰⁰ Rückfahrt Salzburg

Bitte melden Sie sich online, per e-mail oder per Fax bis zum 31. Juli 2011 an.
Bitte geben Sie auch an, ob Sie an der Führung durch den FRM II (gültiger Personalausweis oder Reisepass erforderlich!) teilnehmen möchten:

TU München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II)
Lichtenbergstraße 1, 85748 Garching (Germany)
Dr. Martin Meven, e-mail martin.meven@frm2.tum.de
Tel. +49 (0)89 28 91 47 27, Fax +49 (0)89 28 91 49 95
www.dgkristall2.de → Arbeitskreise → AK7 → Aktivitäten

For detailed information and registration, please refer to www.salzburg2011.org.

Monday, 19 September 2011

07⁰⁰–19⁰⁰

Leaders

Tungsten deposit Felbertal, Salzburg, Austria

J. G. Raith (Leoben/AT), S. Schmidt (Mittersill/AT)

The scheelite deposit Felbertal, located south of Mittersill, Salzburg province, Austria, is one of the biggest producing tungsten mines in the world. It has long been regarded as the type locality of strata-bound tungsten deposits although the genetic concepts (syngenetic exhalative-hydrothermal vs. granite-related magmatic hydrothermal) and the age of mineralisation are still debated.

Key features of tungsten mineralisation and its geological setting will be seen on this excursion and the genesis of this ore deposit will be re-evaluated on the basis of new mineralogical, geochemical and geochronological data.

Time: 06³⁰–19⁰⁰

Fee Student: 60 EUR

Fee Regular: 75 EUR

Max. number of participants: 14

Monday, 19 September 2011

08⁰⁰–20⁰⁰

Leader

Variscan granites in the Bohemian Massif

F. Finger (Salzburg/AT)

On this excursion you will visit granite outcrops and anatexes on the southern edge of the Bohemian Massif. General questions on the formation and classification as well as possible causes for the striking granite activity in the Bohemian Massif will be answered.

Time: 08³⁰–20⁰⁰

Fee: 30 EUR

Max. number of participants: 30

Saturday, 24 September 2011

07⁰⁰–19⁰⁰

Leaders

Alpine Metamorphism in the Tauern Window – Großglockner cross-section

E. Dachs (Salzburg/AT), A. Proyer (Graz/AT)

The excursion route will follow the Großglockner-High-Alpine Road through the lithologies of the Glockner- und Seidlwinkl Nappe. The effects of Alpine metamorphism (Eoalpine high-pressure metamorphism and 'Tauern-crystallization') will be shown and discussed using selected outcrops.

Time: 07³⁰–19⁰⁰

Fee: 30 EUR

Max. number of participants: 20

Plenary Talks

Wednesday, 21 September 2011

- 09⁰⁰–10⁰⁰ **“Small is Strong” – towards a quantitative understanding of deformation behavior at the micro- and nano-scale**
G. Dehm (Leoben/AT)
- 14⁰⁰–15⁰⁰ **Chemical variations in ‘calckaline’ granitic magmas – neither mixing nor fractionation**
J.D. Clemens (Stellenbosch/ZA)
- 20⁰⁰–21⁰⁰ **High T_c superconductivity – after a quarter century – ready for take-off**
J.G. Bednorz (Zurich/CH)

Thursday, 22 September 2011

- 09⁰⁰–10⁰⁰ **Modern laboratory X-ray powder diffraction – The synchrotron’s poor cousin or powerful research tool?**
P. Whitfield (Ottawa/CA)
- 14⁰⁰–15⁰⁰ **Molecular mechanisms of RNA degradation**
E. Conti (Munich/DE)

Friday, 23 September 2011

- 09⁰⁰–10⁰⁰ **Mineralsimulationen für die Photovoltaik und Thermoelektrik**
K. Bente (Leipzig/DE)
- 10⁰⁰–11⁰⁰ **The economic mineralogy of high-tech metals**
F.M. Meyer (Aachen/DE)

13⁰⁰–16⁰⁰
HS 414

DMG Board Meeting

13⁰⁰–16⁰⁰
HS 421

DGK Board Meeting

16⁰⁰–17⁰⁰
HS 401

Opening
Welcome Notes

G. Amthauer (Salzburg/AT), Conference chair
H. Schmidinger (Salzburg/AT), Rector of the University of Salzburg
H. Dittrich (Salzburg/AT), Chairman of the Dept. for Materials Research & Physics
U. Heinemann (Berlin/DE), President of the DGK
R. Altherr (Heidelberg/DE), President of the DMG
V. Kahlenberg (Innsbruck/AT), President of the ÖMG

17⁰⁰–17¹⁵

Break

17¹⁵–19¹⁵
HS 401

Awards 2011 and award-lectures of 2010

Victor Moritz Goldschmidt Prize 2010
From first-principles to geological processes
S. Jahn (Potsdam/DE)

Felix Machatschki Prize 2010
Open Min(d)
R. Krickl (Vienna/AT)

Max von Laue Prize 2010
From thorium to curium – a structural diversity of actinide borates
E.V. Alekseev (Jülich/DE)

from 19¹⁵

Get-Together (see page 59)

Scientific Programme • Wednesday, 21 September 2011

- 09⁰⁰–10⁰⁰
HS 401
Speaker
Convener
- “Small is Strong” – towards a quantitative understanding of deformation behavior at the micro- and nano-scale**
G. Dehm (Leoben/AT)
H. Dittrich (Salzburg/AT)
- 10⁰⁰–10³⁰
Coffee Break
- 10³⁰–12³⁰
HS 401
Convener
- MS 1: Crystallography at High Pressure/Temperature**
N. Dubrovinskaia, L. Dubrovinsky (Bayreuth/DE)
- 10³⁰
MS01–T1
- Single crystal X-ray diffraction at megabar pressures and temperatures of thousands degrees – from geosciences to materials**
L. Dubrovinsky, K. Glazyrin, T. Boffa-Ballaran, E. Bykova, N. Dubrovinskaia
M. Merlini (Bayreuth/DE), M. Hanfland (Grenoble/FR)
- 10⁴⁵
MS01–T2
- The shock-wave-synthesis laboratory at the Freiberg high-pressure research centre**
K. Keller, T. Schlothauer, M. Schwarz, G. Heide, E. Kroke (Freiberg/DE)
- 11⁰⁰
MS01–T3
- Anomalies and phase transitions of dense ice**
R. Caracas (Lyon/FR), R.J. Hemley (Washington, DC/US)
- 11¹⁵
MS01–T4
- New insight into boron phases and their relations under pressure**
N. Dubrovinskaia, G. Parakhonskiy, L. Dubrovinsky (Bayreuth/DE)
- 11³⁰
MS01–T5
- High pressure behavior of α -FeOOH studied on powder and single crystal samples**
E. Bykova (Bayreuth/DE), E. Greenberg (Tel-Aviv/IL), K. Glazyrin, T. Boffa Ballaran
N. Dubrovinskaia, L. Dubrovinsky (Bayreuth/DE)
- 11⁴⁵
MS01–T6
- The fluorescence lifetime of $\text{SrB}_4\text{O}_7\text{:Sm}^{2+}$ at high pressures and temperatures**
J. Bauer, L. Bayarjargal, B. Winkler (Frankfurt a.M./DE)
- 12⁰⁰
MS01–T7
- Synthesis of novel ultra-incompressible rhenium nitrides by reaction of the elements in the laser-heated diamond anvil cell and characterization**
A. Friedrich, B. Winkler, W. Morgenroth, L. Bayarjargal (Frankfurt a.M./DE)
E.A. Juarez-Arellano (Tuxtepec/MX), K. Refson (Didcot/GB)
V. Milman (Cambridge/GB)
- 12¹⁵
MS01–T8
- High-pressure crystal structure and Raman spectra of $\text{Bi}_{12}\text{TiO}_{20}$ sillenite**
L. Wiehl, A. Friedrich, W. Morgenroth, E. Haussühl, B. Winkler (Frankfurt a.M./DE)

10 ³⁰ –12 ³⁰ HS 402 Convener	MS 2: Functional Materials I K. Bente (Leipzig/DE), H. Dittrich (Salzburg/AT)
10 ³⁰ MS02–T1	Sr₃Gd₂[BO₃]₄– growth, structure and analyses of a not so new borate <u>Ch. Reuther</u> , H. Schmidt, M. Hengst, G. Heide (Freiberg/DE)
10 ⁴⁵ MS02–T2	Strange high temperature characteristics of GdCa₄O(BO₃)₃ – single crystals for high temperature piezoelectric applications <u>R. Möckel</u> , M. Hengst, M. Klinger, J. Götze, G. Heide (Freiberg/DE)
11 ⁰⁰ MS02–T3	Besonderheiten der Mn-Fixierung in Perowskiten Ca(Al,Fe,Mn,Ti)O₃-d <u>S. Stöber</u> (Halle, Saale/DE), G. Redhammer (Salzburg/AT), H. Pöhlmann (Halle, Saale/DE)
11 ¹⁵ MS02–T4	Deposition of sulfosalt thin films for photovoltaic application <u>J. Stöllinger</u> , H. Dittrich (Salzburg/AT)
11 ³⁰ MS02–T5	Thermoelektrisch und photovoltaisch relevante Dünnschichten und Whisker im System SnS-PbS <u>R. Kaden</u> , G. Wagner, D. Unuchak, K. Bente (Leipzig/DE)
11 ⁴⁵ MS02–T6	Kesterite type semiconductors for thin film solar cells S. Schorr (Berlin/DE)
12 ⁰⁰ MS02–T7	Crystal growth and properties of semiconducting sulfosalts in the Ag₂S-PbS-Bi₂S₃ system <u>S. Lobe</u> , K. Bente, G. Wagner, R. Kaden (Leipzig/DE)
12 ¹⁵ MS02–T8	Al-doped zincite (ZnO:Al) thin films for transparent conductive oxide applications <u>A. Stadler</u> , J. Stoellinger, H. Dittrich (Salzburg/AT)

- 10³⁰–12³⁰
HS 403
Convener
- MS 3: Metamorphic and Magmatic Processes I**
F. Finger, E. Dachs (Salzburg/AT)
- 10³⁰
MS03–T1
Keynote
- Fluids and charnockite formation during high-grade granulite-facies metamorphism in southern India**
D. Harlov (Potsdam/DE)
- 10⁴⁵
MS03–T2
- EMP monazite age dating enhanced with automated mineralogical methods and it's application in the polymetamorphic Saualpe basement (Eastern Alps)**
B. Schulz (Freiberg/DE)
- 11⁰⁰
MS03–T3
- Formation and alteration of zircons in archaean granitoids from Swaziland combined insights from CL-imaging, trace element, $\delta^{18}\text{O}$, U-Th-Pb and Lu-Hf isotope analyses**
A. Zeh, A. Gerdes, R. Stern (Frankfurt a.M./DE)
- 11¹⁵
MS03–T4
- Fluid-mediated equilibration and self-irradiation in complex euxenite-zircon assemblages of pegmatites from South Norway – implications for U-Pb geochronology**
A.-M. Seydoux-Guillaume, C. Duran, B. Bingen, P. de Parseval
D. Guillaume (Toulouse/FR), V. Bosse, J.-L. Paquette (Clermont-Ferrand/FR)
J. Ingrin (Lille/FR)
- 11³⁰
MS03–T5
- Modeling magma differentiation processes in volcanic systems – key examples from Klyuchevskoy, Bezymianny and Mutnovsky volcanoes, Kamchatka**
R. Almeev (Hanover/DE), A. Ariskin (Moscow/RU), R. Botcharnikov, F. Holtz
T. Shishkina (Hanover/DE), M. Portnyagin (Kiel/DE), J.-I. Kimura (Yokosuka/JP)
A. Ozerov (Petropavlovsk-Kamchatsky/RU)
- 11⁴⁵
MS03–T6
- Domain structure in fine-grained orthopyroxene-plagioclase-spinel symplectite in basanite hosted mantle xenoliths from Zinst (Bavaria)**
G. Habler, R. Abart (Vienna/AT), P. Spacek (Prague/CZ)
- 12⁰⁰
MS03–T7
- Plagioclase-bearing mantle lherzolites from the central dinaridic ophiolite zone (CDOB, NE Bosnia and Herzegovina) – evidences of upper mantle metasomatism**
B. Segvic (Darmstadt/DE), R. Altherr (Heidelberg/DE)
- 12¹⁵
MS03–T8
- Solubility of Au and Mo in volatile-bearing magmas**
R. Botcharnikov (Hanover/DE), R. Linnen (London/GB), F. Holtz (Hanover/DE)
M. Wilke (PotsdamDE)

10 ³⁰ –12 ⁰⁰ HS 434 Convener	MS 4: Computational Crystallography G. Raabe (Aachen/DE), S. Gemming (Dresden/DE)
10 ³⁰ MS04–T1	Spin transition in Fe-bearing perovskite – implications for the lower mantle R. Caracas (Lyon/FR)
10 ⁴⁵ MS04–T2	Orbital ordering in the ferromagnetic phase of the kagome staircase compound $\text{Co}_3\text{V}_2\text{O}_8$ N. Narayanan (Darmstadt/DE), N. Qureshi (Cologne/DE), H. Fuess (Darmstadt/DE) H. Ehrenberg (Karlsruhe/DE)
11 ⁰⁰ MS04–T3	Surface energy and bond energy calculations of fcc- and bcc- metals by application of the bond deficiency model A. Mutter (Kiel/DE), L. Peters (Aachen/DE)
11 ¹⁵ MS04–T4	Crystal structure prediction as tool for crystal engineering of co-crystals – the prediction of free lattice energies and its effect on thermodynamic properties, e.g. solubility L.N. Kuleshova, D.W.M. Hofmann (Pula/IT)
11 ³⁰ MS04–T5	New developments on the Bilbao crystallographic server M.I. Aroyo, J.M. Perez-Mato, D. Orobengoa, E.S. Tasci, G. de la Flor S. V. Gallego (Bilbao/ES)
11 ⁴⁵ MS04–T6	Data base driven crystal structure prediction with fine-tuned force fields D.W.M. Hofmann (Uttenreuth/IT), L.N. Kuleshova (Pula/IT) F. Hofmann (Erlangen-Nürnberg/DE)
12 ³⁰ –14 ⁰⁰	Lunch Break
12 ⁴⁵ –13 ⁴⁵ HS 402	Lunch Symposium Bruker AXS Integrated solutions – as individual as your research*
14 ⁰⁰ –15 ⁰⁰ HS 401 Speaker Convener	Chemical variations in ‘calcalkaline’ granitic magmas – neither mixing nor fractionation J.D. Clemens (Stellenbosch/ZA) W. Heinrich (Potsdam/DE)



* Snacks and beverages will be served.

- 16⁰⁰–18⁰⁰
HS 401
Convener M. Meven (Munich/DE), G. Redhammer (Salzburg/AT)
MS 5: Synchrotron- and Neutron Diffraction
- 16⁰⁰
MS05-T1
The upgrade programme of the structural biology beam lines at the european synchrotron radiation facility (ESRF)
Ch. Mueller-Dieckmann (Grenoble/FR)
- 16¹⁵
MS05-T2
A sapphire single crystal cell for neutron powder diffraction at high gas pressures
H. Kohlmann, N. Kurtzemann, C. Reichert, P. Wenderoth (Saarbrücken/DE)
- 16³⁰
MS05-T3
Room temperature single-crystal diffuse scattering and ab initio lattice dynamics in titanite, CaTiSiO₅
M. Gutmann, K. Refson (Chilton Didcot/GB), M. von Zimmermann (Hamburg/DE)
I. Swainson (Ottawa/CA), H. Dabkowska, A. Dabkowski (Hamilton/GB)
- 16⁴⁵
MS05-T4
Magnetic and low temperature structural behavior of clinopyroxene-type FeGeO₃ – a neutron diffraction, magnetic susceptibility and ⁵⁷Fe Mössbauer study
G. Redhammer (Salzburg/AT), A. Senyshyn (Garching/DE), G. Tippelt (Salzburg/AT)
W. Treutmann, C. Pietzonka (Marburg a.d. Lahn/DE), G. Roth (Aachen/DE)
G. Amthauer (Salzburg/AT)
- 17⁰⁰
MS05-T5
Characterizing the main hardening TaC precipitates by complementary diffraction methods in high melting Co-Re base alloys being developed for applications at temperatures beyond the Ni-base superalloys
R. Gilles (Munich/DE), D. Mukherji (Braunschweig/DE), P. Strunz (Prague/CZ)
M. Hofmann, M. Hoelzel (Munich/DE), B. Barbier, H. Euler (Bonn/DE)
J. Rösler (Braunschweig/DE), U. Gasser (Villigen/CH)
- 17¹⁵
MS05-T6
Crystal structure of Li₂B₄O₇
A. Senyshyn (Darmstadt/DE), H. Boysen (Garching/DE), R. Niewa (Stuttgart/DE)
Y. Burak, V. Adamiv (Lviv/UA), I. Chumak (Dresden/DE), H. Fuess (Darmstadt/DE)
- 17³⁰
MS05-T7
Native point defects in CuGaSe₂ – a structural study based on the complementary use of synchrotron X-rays and neutrons
C. Stephan, S. Schorr, T. Scherb (Berlin/DE)
- 17⁴⁵
MS05-T8
High resolution investigations of cementitious materials by synchrotron radiation based X-ray diffraction
M.-C. Schlegel, U. Mueller, U. Panne, F. Emmerling (Berlin/DE)

- 16⁰⁰–18⁰⁰
HS 402
Convener
- MS 6: Functional Materials II and Ionic Conductors**
K. Bente (Leipzig/DE), H. Dittrich (Salzburg/AT)
- 16⁰⁰
MS06–T1
- Crystal chemistry and stability of Li₇La₃Zr₂O₁₂ garnet – a fast lithium-ion conductor**
C.A. Geiger (Salzburg/AT), E. Alekseev (Jülich/DE), B. Lazic, M. Fisch
T. Armbruster (Bern/CH), R. Langner, M. Fechtelkord (Bochum/DE)
N. Kim (Stanford, CA/US), T. Pettke (Bern/CH), W. Weppner (Kiel/DE)
- 16¹⁵
MS06–T2
- Raman-Spektroskopie diamantähnlicher Kohlenstoffbeschichtungen für funktionelle Oberflächen**
M. Kahn (Villach/AT), R. Kaindl, W. Waldhauser (Niklasdorf, Villach/CH)
- 16³⁰
MS06–T3
- Microstructures of coke deposits from high temperature processes**
S. Gerhardt, K. Bente, J. Hofmann (Leipzig/DE)
- 16⁴⁵
MS06–T4
- Flexible single-crystal media for dynamic separation of gas**
S. Takamizawa (Yokohama/JP)
- 17⁰⁰
MS06–T5
- Fabrication and characterization of piezoceramics from lead based and lead free systems**
M. Prakasam, A. Largeau, P. Veber, M. Maglione, E.A.Villora
K. Shimamura (Pessac, Bordeaux/FR)
- 17¹⁵
MS06–T6
- In search of Li-Na-ionic conductors**
S. Park, J. Labbe, I.F. Akter, C.J. Pietsch, L. Garcia, B. Lara (Munich/DE)
- 17³⁰
MS06–T7
- Synthesis and properties of NaBH₄-imbibed aluminosilicate gels and its partial crystalline secondary products**
J.-Ch. Buhl (Hanover/DE)
- 17⁴⁵
MS06–T8
- Hydrogen release and reinsertion reactions in (BH_x-(OH)_y-O_z)-SOD zoned crystal systems**
C. Rüschler, L. Schomborg, J.-C. Buhl (Hanover/DE)

- 16⁰⁰–17¹⁵
HS 403
Convener **MS 7: Metamorphic and Magmatic Processes II and Thermodynamics**
F. Finger, E. Dachs (Salzburg/AT)
- 16⁰⁰
MS07–T1 **Modification of meteoritic tracer element ratios during projectile and target interaction in laser and hypervelocity experiments**
L. Hecht, M. Ebert (Berlin/DE), A. Deutsch (Münster/DE), T. Kenkmann (Freiburg/DE)
- 16¹⁵
MS07–T2 **Li and B equilibrium isotope fractionation between minerals and aqueous solution from first principles calculations**
P. Kowalski, S. Jahn, B. Wunder (Potsdam/DE)
- 16³⁰
MS07–T3 **Understanding peralkaline magmatic systems – an experimental approach**
Ch. Giehl, M. Marks, M. Nowak (Tübingen/DE)
- 16⁴⁵
MS07–T4 **Water-rock interaction in high pressure MOR hydrothermal systems – an experimental approach for in situ sampling of coexisting brine and vapour phases up to 550 bar and 500°C**
O. Beermann, D. Garbe-Schönberg, A. Holzheid, C. Kusebauch (Kiel/DE)
- 17⁰⁰
MS07–T5 **Solubility measurements of CePO₄ and YPO₄ in H₂O–NaF at 800°C and 1 GPa: implications for extremely high REE transport during granulite-facies metamorphism**
P. Tropper (Innsbruck/AT), C. Manning, D. Harlov (Los Angeles, CA/US)

16 ⁰⁰ –16 ⁴⁵ HS 434 Convener	MS 8: Archeomaterials S. Klein (Frankfurt a.M./DE)
16 ⁰⁰ MS08–T1	Kunstgeschichtlich bedeutsame Ockerpigmente aus Thüringen – Bergbau, Mineralogie und Geochemie <u>E. Knop</u> (Salzburg/AT), A. Karstädt (Erfurt/DE), V. Gröschner (Rudolstadt/DE)
16 ¹⁵ MS08–T2	Provenancing classical marbles with object based image analysis P. Hofmann, <u>R. Marschallinger</u> , M. Unterwurzacher, F. Zobl (Salzburg/AT)
16 ³⁰ MS08–T3	MS-TG Analysis – a method to detect volatile impurities <u>K. Galonska</u> , G. Heide (Freiberg/DE)
16 ⁴⁵ –17 ⁰⁰	Break
17 ¹⁵ –18 ¹⁵ HS 403 Convener	MS 9: Thermodynamics and Energetics of Earth Materials E. Dachs (Salzburg/AT)
17 ¹⁵ MS09–T1	Thermodynamic properties of grossular garnet I – nature of problem, analysis of published calorimetric data and sample characterization <u>C.A. Geiger</u> , E. Dachs (Salzburg/AT)
17 ³⁰ MS09–T2	Thermodynamic properties of grossular garnet II – heat capacity measurements and behavior, standard entropy and selected petrologic applications <u>C.A. Geiger</u> , E. Dachs (Salzburg/AT)
17 ⁴⁵ MS09–T3	Symplectite formation in the CaO-MgO-SiO₂ system – experiments and thermodynamic model <u>R. Abart</u> , B. Joachim (Vienna/AT), P. Remmert (Potsdam/DE), G. Habler (Vienna/AT) R. Wirth (Potsdam/DE)
18 ⁰⁰ MS09–T4	First-principles thermodynamics of oxides and silicates in the Mg-Si-O system: application to phase equilibria calculation at high pressures and temperatures <u>D. Belmonte</u> , G. Ottonello, M. Vetuschi Zuccolini (Genova/IT)

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17 ⁰⁰ –18 ⁰⁰ HS 434 Convener	MS 10: Mineralogy at School R. Stalder (Innsbruck/AT)
17 ⁰⁰ MS10–T1	Sichtbarkeit der Mineralogie in unserer Gesellschaft – ein Spiegelbild unseres Schulsystems R. Stalder (Innsbruck/AT)
17 ¹⁵ MS10–T2	Vom Lehrplan bis zur Schulbuchgenehmigung – der Weg naturwissenschaftlicher Inhalte in den Unterricht W. Schierle (Heilbronn/DE)
17 ³⁰ MS10–T3	Schulgeographie 2000 plus – mit den Geowissenschaften durchs neue Millennium!? G. Falk (Freiburg/DE)
17 ⁴⁵ MS10–T4	Unkonventionell und unerlässlich – Mineralogie im Schulalltag <u>D. Jacob</u> , S. Horn (Mainz/DE)
18 ⁰⁰	Discussion
18 ¹⁵ –19 ⁴⁵ HS 402	DGK Members Meeting
20 ⁰⁰ –21 ⁰⁰ HS 401 Speaker Convener	High T_c superconductivity – after a quarter century – ready for take-off J.G. Bednorz (Zurich/CH) U. Heinemann (Berlin/DE)

- 09⁰⁰–10⁰⁰
 HS 401
 Speaker P. Whitfield (Ottawa/CA)
 Convener N. Hüsing (Salzburg/AT)
- 10⁰⁰–10³⁰
 Coffee Break
- 10³⁰–12³⁰
 HS 401
 Convener N. Hüsing (Salzburg/AT), M. Weil (Vienna/AT)
- 10³⁰
 MS11–T1
ICSD Web – current state and new developments
 S. Rühl (Eggenstein-Leopoldshafen/DE)
- 10⁴⁵
 MS11–T2
Fascinating structural and topological complexity of oxocentered units in divalent lead natural and synthetic oxyhalides
O. Siidra, S. Krivovichev (Saint-Petersburg/RU)
- 11⁰⁰
 MS11–T3
Multi-valence states and multi-coordinations in complex actinide phosphites and phosphates
E.V. Alekseev (Kiel/DE), E.M. Villa (Notre Dame/FR), W. Depmeier (Kiel/DE)
 T.E. Albrecht-Schmitt (Notre Dame/FR)
- 11¹⁵
 MS11–T4
Lanthanido-ammonium cations [NLn₄]⁹⁺ as prominent structural features in nitride derivatives of the 4f-elements
T. Schleid, F. Lissner (Stuttgart/DE)
- 11³⁰
 MS11–T5
Das Rätsel der „ungeordneten“ Turmaline
A. Ertl, E. Tillmanns (Vienna/AT)
- 11⁴⁵
 MS11–T6
Straight Si–O–Si bond angles at low temperature
 H. Effenberger (Vienna/AT)
- 12⁰⁰
 MS11–T7
BaPO₃F and β-Hg₂CrO₄ – structural relations explained by order-disorder (OD) theory
B. Stöger, M. Weil (Vienna/AT)
- 12¹⁵
 MS11–T8
Disorder in crystalline compounds investigated by a combination of X-ray diffraction, NMR spectroscopy, and DFT calculations
 F. Haarmann (Aachen/DE)

- 10³⁰–12¹⁵
HS 402
Convener **MS 12: Functional Materials III (CSH-Phases and Phosphates)**
K.T. Fehr, R. Hochleitner (Munich/DE)
- 10³⁰
MS12–T1
Keynote **Reaction kinetics of the 1.13 nm tobermorite formation – new insights on rate constants and activation energies by in-situ-neutron diffraction experiments**
S. Bernstein (Rohrdorf/DE)
- 11⁰⁰
MS12–T2 **A natural CSH-laboratory – CSH-phases and their parageneses from Maroldsweisach, Bavaria**
R. Hochleitner, K.T. Fehr (Munich/DE)
- 11¹⁵
MS12–T3 **Time resolved in-situ XRD-analysis of the evolution of C-S-H gel during the early hydration of alite with water**
S. Bergold, D. Jansen, F. Goetz-Neunhoeffer, J. Neubauer (Erlangen/DE)
- 11³⁰
MS12–T4 **A model of OPC hydration based on pore solution equilibria – highly timeresolved monitoring of cement hydration using synchrotron X-radiation**
I. Mueller (Burghausen/DE)
- 11⁴⁵
MS12–T5 **Identification and quantification of phosphate mineral phases generated by CSH-seeded crystallization from sewage**
A. Ehbrecht, R. Schuhmann, T. Fuderer, S. Schönaier (Eggenstein-Leopoldshafen/DE)
- 12⁰⁰
MS12–T6 **Comparison of phospho-olivines as cathode materials in rechargeable Li-ion batteries**
A. Laumann, N. Tran, G. Nuspl, N. Schall (Moosburg/DE)

- 10³⁰–12¹⁵
HS 403
Convener **MS 13: Mineral Resources for High-Tech Materials**
F. M. Meyer (Aachen/DE), T. Oberthür (Hanover/DE)
- 10³⁰
MS13–T1 **Metasediment hosted synorogenic cobalt-copper-gold (-nickel) mineralization in the Siegerland-Wied district of the Variscan fold-and thrust belt, Rhenish Massif**
A. Hellmann, F.M. Meyer, A. Cormann, M. Peters (Aachen/DE)
- 10⁴⁵
MS13–T2 **The LREE-, Se- and Au- bearing BiCoNi-U-Ag-association of the Schlema-Alberoda-complex U-deposit**
T. Schlothauer, A.D. Renno, G. Bombach, G. Heide, W. Klemm (Freiberg/DE)
- 11⁰⁰
MS13–T3 **Trace elements in cassiterite and wolframite**
S. Goldmann, F. Melcher, H.-E. Gäbler (Hanover/DE)
- 11¹⁵
MS13–T4 **Trace elements in Ta-Nb oxides from granitic and pegmatitic tantalum provinces**
F. Melcher, H.-E. Gäbler, T. Graupner, M. Sitnikova (Hanover/DE)
- 11³⁰
MS13–T5 **Classification of REE distribution patterns of CGM**
T. Graupner, F. Melcher, H.-E. Gäbler, M. Sitnikova (Hanover/DE)
- 11⁴⁵
MS13–T6 **The caeiras-pegmatite – a new occurrence and its potential for high-tech-metals in the Borborema Pegmatite Province, NE-Brazil**
S. Sindern, C. Piribauer, F. M. Meyer, D. Mashev, V. Havenith (Aachen/DE)
R.F.S. Lima, R.A. Petta, T.F.C. Campos (Natal, RN/BR), R.J. Bakker (Leoben/AT)
- 12⁰⁰
MS13–T7 **The potential of rare earth elements in the Co-rich ferromanganese crust deposits of the pacific ocean**
A. Jahn, P. Halbach (Berlin/DE)

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- 10³⁰–12³⁰
HS 434
Convener
- MS 14: Bio-Crystallography I**
R. Ficner (Göttingen/DE), J. Brandstetter (Salzburg/AT)
- 10³⁰
MS14–T1
- Let's twist – unexpected geometry of Schiff-base intermediates and protein dynamics in transaldolase**
A. Lehwiss-Litzmann, P. Neumann (Göttingen/DE), C. Parthier (Halle, Saale/DE)
S. Lüdtke (Göttingen/DE), R. Golbik (Halle, Saale/DE), R. Ficner
K. Tittmann (Göttingen/DE)
- 10⁵⁰
MS14–T2
- Structure and mechanism of chloromomuconolactone dehalogenase from *rhodococcus opacus* TCP**
Ch. Roth, S.R. Kaschabek (Leipzig, Freiberg/DE), J.A.D. Gröning
M. Schlömann (Freiberg/DE), N. Sträter (Leipzig/DE)
- 11¹⁰
MS14–T3
- Crystal structure of NirE in complex with its substrate reveals new insights into the catalytic mechanism of SUMT enzymes**
S. Saha, S. Storbeck, J. Krausze, B.U. Klink, D.W. Heinz, G. Layer (Braunschweig/DE)
- 11³⁰
MS14–T4
- Structures of *physcomitrella patens* AOC1 and AOC2 complexes reveal unexpected conformation of the epoxide ring of the bound substrate analogs**
P. Neumann, K. Sauer, J. Brinkmann, F. Brodhun, A. Dickmanns, I. Feussner
R. Ficner (Göttingen/DE)
- 11⁵⁰
MS14–T5
- Structure of human dipeptidyl peptidase III in complex with an opioid peptide unveils an unusual entropy-driven binding mode**
G. Arruda Bezerra (Graz/AT), M. Abramic (Zagreb/HR), P. Macheroux (Graz/AT)
S. Dhe-Paganon (Toronto/CA), K. Gruber (Graz/AT)
- 12¹⁰
MS14–T6
- Unusual carbon fixation giving rise to diverse polyketideextender units**
N. Quade (Braunschweig/DE), L. Huo (Saarbrücken/DE)
D.W. Heinz (Braunschweig/DE), R. Müller (Saarbrücken/DE)
- 12³⁰–14⁰⁰
- Lunch Break
- 12⁴⁵–13⁴⁵
HS 402
- Lunch Symposium FEI Company**
Multi-scale, multi-dimensional imaging of earth materials
- 14⁰⁰–15⁰⁰
HS 401
Speaker
Convener
- Molecular mechanisms of RNA degradation**
E. Conti (Munich/DE)
J. Brandstetter (Salzburg/AT)



- 16⁰⁰–18⁰⁰
HS 401
Convener
- MS 15: Inorganic Structures II**
N. Hüsing (Salzburg/AT), M. Weil (Vienna/AT)
- 16⁰⁰
MS15–T1
- High-pressure phase transformation of SiO₂ polymorphs to Seifertite**
U. Bläß, F. Langenhorst (Jena/DE)
- 16¹⁵
MS15–T2
- High pressure synthesis of single crystals of α-boron**
G. Parakhonskiy, N. Dubrovinskaia, L. Dubrovinskiy, S. Mondal
S. van Smaalen (Bayreuth/DE)
- 16³⁰
MS15–T3
- Symmetry mode based parametric Rietveld refinement applied to structural phase transitions**
M. Müller (Trento/IT), R. Dinnebier (Stuttgart/DE), S. Schorr (Berlin/DE)
- 16⁴⁵
MS15–T4
- Crystal orientation investigation of Japanese twins in quartz using EBSD**
A. Lenart, Z. Samardžija, M. Gec, B. Mirtič, S. Šturm (Ljubljana/SI)
- 17⁰⁰
MS15–T5
- A⁵⁷Fe Mössbauer study of local structure and cation distribution in mullite-type Bi₂(Fe_xMn_{1-x})₄O₁₀ and in Bi₂(Fe_xM_{1-x})₄O₉, M=Al, Ga, Mn**
S.-U. Weber (Braunschweig/DE), T.M. Gesing (Bremen/DE)
M. Lufaso (Jacksonville, FL/US), H. Schneider (Köln/DE)
K.-D. Becker (Braunschweig/DE)
- 17¹⁵
MS15–T6
- Dehydration studies of cation-exchanged natrolites**
K. Hoffmann, R.X. Fischer (Bremen/DE)
- 17³⁰
MS15–T7
- Zum Dehydratationsverhalten von Zeolithen – Tieftemperatur-Untersuchungen an Paulingit**
A. Bieniok, P. Göttig, U. Brendel (Salzburg/AT)
- 17⁴⁵
MS15–T8
- Highly symmetric complex intermetallics**
J. Dshemuchadse, D.Y. Jung, W. Steurer (Zurich/CH)

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- 16⁰⁰–16⁴⁵
HS 402
Convener
MS 12: Functional Materials III (CSH-Phases and Phosphates)
K.T. Fehr, R. Hochleitner (Munich/DE)
- 16⁰⁰
MS12–T7
Behavior of lithium during the topotactic formation of ferrisicklerite from triphylite
P. Schmid-Beurmann (Münster/DE), T. Geisler (Bonn/DE), F. Hatert (Liège/BE)
L. Ottolini (Pavia/IT), D.M. Többens, V. Kahlenberg (Innsbruck/AT)
- 16¹⁵
MS12–T8
Glimpses at individual reaction steps accompanying the crystallization of the tridymite form(s) of AlPO₄ from an X-ray amorphous precipitate doped with potassium and magnesium
B. Peplinski, B. Adamczyk, C. Adam, F. Emmerling (Berlin/DE)
- 16³⁰
MS12–T9
Crystallochemical investigations in the join Plumbojarosite – Corkite – Kintoreite
R. Hochleitner, C. Rewitzer, M. Kaliwoda, K.T. Fehr (Munich/DE)
- 16⁰⁰–16⁴⁵
HS 403
Convener
MS 16: New Methods in Analyses of Mineral Resources
J.G. Raith (Leoben/AT), F. Melcher (Hanover/DE)
- 16⁰⁰
MS16–T1
U-Pb dating of scheelite by LA-SF-ICP-MS constrains the variscan age of the Felbertal tungsten deposit
J.G. Raith (Leoben/AT), A. Gerdes (Frankfurt a.M./DE), D. Cornell (Gothenburg/DE)
- 16¹⁵
MS16–T2
Proof of origin of coltan ores by in-situ microanalytical methods – MLA and SF-LA-ICP MS
M. Sitnikova, E. Gäbler, T. Graupner, F. Melcher (Hanover/DE)
- 16³⁰
MS16–T3
Fractionation of the Lu-Hf isotope system during formation of Nb-Ta mineralisations
A. Gerdes, L. Marko (Frankfurt a.M./DE), F. Melcher (Hanover/DE)
- 16⁴⁵–17⁰⁰
Break

- 16⁰⁰–18⁴⁰
HS 434
Convener
- MS 17: Bio-Crystallography II**
R. Ficner (Göttingen/DE), J. Brandstetter (Salzburg/AT)
- 16⁰⁰
MS17-T1
- Structure and biochemical analysis of alzheimer's disease amyloid precursor protein (APP)**
M. Than, S.O. Dahms, S. Hoefgen, I. Könnig, D. Roeser (Jena/DE)
- 16²⁰
MS17-T2
- The structure of collagenase G at 2.55 angström resolution reveals a chew & digest mechanism of bacterial collagenolysis**
U. Eckhard, E. Schönauer, D. Nüss, H. Brandstetter (Salzburg/AT)
- 16⁴⁰
MS17-T3
- The structural basis of proteolysis and host-pathogen interaction by pestivirus protein Npro**
I. Zögg (Salzburg/AT), M. Sponring, M. Koll, R. Schneider (Innsbruck/AT)
H. Brandstetter (Salzburg/AT), B. Auer (Innsbruck/AT)
- 17⁰⁰
MS17-T4
- Cap architecture conservation in monoglyceride lipases from bacteria to humans**
M. Oberer, S. Rengachari, G. Arruda Bezerra, C. Sturm, L. Riegler, C.C. Gruber
U. Taschler, A. Boeszoermenyi, R. Zimmermann, K. Gruber (Graz/AT)
- 17²⁰
MS17-T5
- Crystal structures of velvet transcription factors reveal an unexpected fold**
Y.L. Ahmed, P. Neumann, Ö. Bayram, J. Gerke, G. Braus, R. Ficner (Göttingen/DE)
- 17⁴⁰
MS17-T6
- X-ray structure refinement with canonical distributions of electrons**
S. Ginzinger, M. Gruber, H. Brandstetter, M. Sippl (Salzburg/AT)
- 18⁰⁰
MS17-T7
- Structural aspects of CRM1 cooperativity – a hybrid methods approach**
A. Dickmanns, N. Doelker (Göttingen/DE), C. Blanchett (Hamburg/DE)
T. Monecke (Göttingen/DE), D. Svergun (Hamburg/DE), R. Ficner
H. Grubmüller (Göttingen/DE)
- 18²⁰
MS17-T8
- Optimal fine ϕ slicing for single photon counting pixel detectors**
M. Mueller (Baden/CH), M. Wang (Villigen-PSI/CH), C. Schulze-Bries (Baden/CH)

- 17⁰⁰–18³⁰
HS 402
Convener **MS 18: Mineral- and Crystal Surfaces**
G. Jordan (Munich/DE)
- 17⁰⁰
MS18–T1 **Interaction of silicic acid with mineral surfaces in the aspects of silicate weathering and adsorption**
M. Dietzel (Graz/AT)
- 17¹⁵
MS18–T2 **Pyrrhotite oxidative dissolution – crystallographic and microstructural controls observed by FIB-TEM and 3D topometry**
D. Harries (Bayreuth/DE), K. Pollok, F. Langenhorst (Jena/DE)
- 17³⁰
MS18–T3 **Citrate induced effects on magnesite growth kinetics**
U.-N. Berninger (Munich/DE), Q. Gautier, J. Schott (Toulouse/FR)
G. Jordan (Munich/DE)
- 17⁴⁵
MS18–T4 **Strontium titanate surface modifications due to nitrogen implantation investigated by grazing incidence XANES**
H. Stöcker, F. Hanzig, J. Seibt, C. Richter, M. Zschornak, D.C. Meyer (Freiberg/DE)
- 18⁰⁰
MS18–T5 **Molecular dynamics simulations of olivine-melt interfaces**
S. Gurmani, S. Jahn, H. Brasse, F.R. Schilling (Potsdam/DE)
- 18¹⁵
MS18–T6 **Grain boundary diffusion in Mg₂SiO₄ forsterite – insights from molecular dynamics simulations**
O. Adjaoud, S. Jahn (Potsdam/DE)

17 ⁰⁰ –18 ¹⁵ HS 403 Convener	MS 19: Environmental Mineralogy and Geochemistry I S. Heuss-Aßbichler (Munich/DE), M. Kersten (Mainz/DE)
17 ⁰⁰ MS19–T1	Secondary phases and surface topography – How can reliable mineral weathering rates be obtained? K. Pollok (Jena/DE)
17 ¹⁵ MS19–T2	Experimentally determined standard properties for synthetic $\text{MgSO}_4 \bullet 4\text{H}_2\text{O}$ (starkeyite) and $\text{MgSO}_4 \bullet 3\text{H}_2\text{O}$; a revised internally consistent thermodynamic dataset for magnesium sulfate hydrates K.-D. Grevel (Bochum/DE), J. Majzlan (Jena/DE), A. Benisek, E. Dachs (Salzburg/AT) M. Steiger (Hamburg/DE), A.D. Fortes (London/GB), B. Marler (Bochum/DE)
17 ³⁰ MS19–T3	Thermodynamics of mixing in barite-celestite solid solution from quantum-mechanical calculations <u>V. Vinograd</u> (Jülich/DE), B. Winkler (Frankfurt a.M./DE), D. Bosbach (Jülich/DE)
17 ⁴⁵ MS19–T4	Raman microprobe analysis and thermodynamic equilibrium modelling of corrosion products formed on depleted uranium ammunition in soil <u>M. Kersten</u> , M. Quadir, T. Häger (Mainz/DE)
18 ¹⁵ –19 ⁴⁵ HS 401	DMG Members Meeting
20 ⁰⁰	Social Evening (see page 59)

Scientific Programme • Friday, 23 September 2011

- 09⁰⁰–10⁰⁰
HS 401
Speaker K. Bente (Leipzig/DE)
Convener G. Amthauer (Salzburg/AT)
Mineralsimulationen für die Photovoltaik und Thermoelektrik
- 10⁰⁰–11⁰⁰
HS 401
Speaker F. M. Meyer (Aachen/DE)
Convener J.G. Raith (Leoben/AT)
The economic mineralogy of high-tech metals
- 11⁰⁰–11¹⁵
Farewell and Outlook Munich 2012
G. Amthauer (Salzburg/AT), W.W. Schmahl (Munich/DE)
- 11¹⁵–11³⁰
Coffee Break
- 11³⁰–13⁰⁰
HS 401
Convener S. Heuss-Abichler (Munich/DE), M. Kersten (Mainz/DE)
MS 20: Environmental Mineralogy and Geochemistry II
- 11³⁰
MS20–T1
D. Klapper, S. Heuss-Abichler (Munich/DE), G. Kochetov, D. Zorya (Kiev/UA)
Characterization of copper minerals recovered from process water
- 11⁴⁵
MS20–T2
J. Majzlan (Jena/DE)
Energetics of well and poorly crystalline arsenates of ferric iron
- 12⁰⁰
MS20–T3
A. Bieniok, U. Brendel, G. Zagler, F. Neubauer (Salzburg/AT)
Sekundär-Mineralisationen aus Karstgebieten im Land Salzburg am Beispiel des Gamslöcher-Kolowrat-Höhlensystems im Untersberg
- 12¹⁵
MS20–T4
K. Beier, A. Holzheid (Kiel/DE)
Results of an experimental study on geochemical behaviors of potential reservoir materials during the CO₂-sequestration process – determination of kinetic data and reasons for their variations
- 12³⁰
MS20–T5
H. Marbler, M. Schmidt, K.P. Erickson, C. Lempp, H. Pöllmann (Halle, Saale/DE)
Geochemical and geomechanical effects on sandstones during the exposure to impure CO₂ – an experimental approach
- 12⁴⁵
MS20–T6
P.M. Kadletz, A.J. Götz, K. Otte, R. Pentcheva, S.-H. Park, W.W. Schmahl (Munich/DE), A. Ziegler (Ulm/DE), F.E. Wagner (Garching/DE), S. Pfeiffer, S. Paikaray (Bayreuth/DE), J. Kipry, C. Wiacek, M. Schlömann (Freiberg/DE), E. Janneck (Halsbrücke/DE)
The structure of schwertmannite and its relevance to ion exchange capabilities for environmental applications

- 11³⁰–13⁰⁰
HS 402
Convener **MS 21: Spectroscopy of Minerals**
A. Beran (Vienna/AT), M. Fechtelkord (Bochum/DE)
- 11³⁰
MS21–T1 **Irradiation effects on the luminescence of monazite**
L. Nasdala (Vienna/AT), D. Grambole (Dresden/DE), K. Ruschel (Vienna/AT)
J.M. Hanchar (St. John's/CA)
- 11⁴⁵
MS21–T2 **Recrystallisation behaviour and structural phenomena of metamict titanite**
T. Beirau, C. Paulmann (Hamburg/DE), U. Kolb, G. Matveeva
I. Andrusenko (Mainz/DE), U. Bismayer (Hamburg/DE)
- 12⁰⁰
MS21–T3 **Combination of raman spectroscopy and electron microprobe within the**
Almahata Sitta meteorite
M. Kaliwoda, R. Hochleitner (Munich/DE), V. Hoffmann (Tübingen/DE)
T. Mikouchi (Tokyo/JP), A.M. Gigler, K.T. Fehr, W.W. Schmahl (Munich/DE)
- 12¹⁵
MS21–T4 **Aluminum ordering and clustering in Al-rich synthetic phlogopite – {¹H} → ²⁹Si**
CPMAS HETCOR spectroscopy and atomistic calculations
M. Fechtelkord, R. Langner (Bochum/DE), A. Garcia (Bellaterra/ES)
E.J. Palin (Cambridge/GB), J. Lopez-Solano (Bilbao/ES)
- 12³⁰
MS21–T5 **Electron channelling spectroscopy of Cr-spinels**
N. Miyajima, W. Sun (Bayreuth/DE)
- 12⁴⁵
MS21–T6 **The WURM project – a web-based freely available database of computed physical**
properties for minerals
R. Caracas, E. Bobocioiu (Lyon/FR)
- 13⁰⁰
MS21–T7 **25 years Mössbauer spectroscopy in Salzburg**
G. Amthauer, M. Grodzicki, W. Lottermoser, G. Redhammer, G. Tippelt (Salzburg/AT)

11 ³⁰ –13 ¹⁵ HS 403 Convener	MS 22: Molecular Chemistry Ch. Lehmann (Mülheim a.d. Ruhr/DE)
11 ³⁰ MS22–T1	Intercluster compounds for nanosized materials <u>F. Gschwind</u> , M. Jansen (Stuttgart/DE)
11 ⁴⁵ MS22–T2	Solid-state versus gas-phase structures of inorganic molecular compounds exhibiting weak correlation driven interactions R.J.F. Berger (Salzburg/AT)
12 ⁰⁰ MS22–T3	Solvate der Cholsäure – nützliche Co-Kristalle <u>U. Englert</u> , R. Wang (Aachen/DE)
12 ¹⁵ MS22–T4	Small changes – big influence – deuterium and fluorine affect crystal packing K. Merz (Bochum/DE)
12 ³⁰ MS22–T5	H-bonding and changes in anion bond lengths B.-C. Nourredine (Khenchela/DZ)
12 ⁴⁵ MS22–T6	Electron densities of balls and bowls <u>P. Luger</u> , D. Lentz, S. Mebs (Berlin/DE), S. Grabowsky (Perth/AU), B. Schmidt M. Weber (Berlin/DE), H. Sakurai, S. Onogi (Myodaiji/JP)
13 ⁰⁰ MS22–T7	Stacking disorder in Pigment Red 170 explained by lattice-energy minimizations <u>J.L. Teteruk</u> , M.U. Schmidt (Frankfurt a.M./DE), T. Gorelik (Mainz/DE) A. Linden (Zurich/CH)

P01	Advances in and beyond Biocrystallography	(see page 38)
P02	Archeomaterials	(see page 38)
P03	Computational and Theoretical Crystallography	(see page 39)
P04	Crystallography at High-Pressure-High-Temperature Conditions – From Minerals to Materials	(see page 39)
P05	Electromechanical and Optical Properties of Solids	(see page 40)
P06	Environmental Mineralogy and Geochemistry	(see page 40)
P07	Enzymes and Mechanisms	(see page 41)
P08	Free Topics	(see page 41)
P09	Functional Materials	(see page 42)
P10	Inorganic Structures	(see page 43)
P11	Ionic Conductors and Hydrogen Storage	(see page 46)
P12	Metamorphic and Magmatic Processes	(see page 46)
P13	Mineral- and Crystal Surfaces	(see page 49)
P14	Mineral Resources for High-Tech Materials	(see page 49)
P15	Molecular Chemistry	(see page 49)
P16	New and Hot Macromolecular Structures	(see page 51)
P17	New Methods in Analyses of Mineral Resources	(see page 51)
P18	Phosphate-Minerals and -Materials	(see page 51)
P19	Promotion of Mineralogy in School Teaching	(see page 52)
P20	Quasi Crystals, Non- and Partial Crystalline Compounds and Modulated Structures	(see page 52)
P21	Spectroscopy of Minerals	(see page 52)
P22	Synchrotron- and Neutron Diffraction	(see page 54)
P23	X-ray powder diffractometry	(see page 54)

- P01** **Advances in and Beyond Biocrystallography**
P01-P01 Experimental phasing using a hexa-sodium α -metatungstate cluster
S.O. Dahms, M. Kuester, M.E. Than (Jena/DE)
- P01-P02 **Facilities for Macromolecular Crystallography at BESSY II – HZB Berlin**
S. Pühringer, M. Bommer, R. Förster, M. Hellmig, M. Krug, K.S. Paithankar, M. Steffien
M. Ühlein, M.S. Weiss, U. Müller (Berlin/DE)
- P02** **Archeomaterials**
P02-P01 Mineralogisch-petrologisch-geochemische Untersuchungen von bronzezeitlichen
Kupferschlacken aus dem Revier Mitterberg
H.-P. Viertler, P. Tropper (Innsbruck/AT)
- P02-P02 Mineralogisch-petrologische Untersuchungen spätbronzezeitlichen Kupferverhüttung
aus dem Revier Mauken (Brixlegg, Tirol)
M. Krismer, M. Tropper, P. Schneider, G. Goldenberg (Innsbruck/AT)
- P02-P03 Mineralogische Charakterisierung der Kupfervererzungen aus der Region Mauken
(Lagerstätte Schwaz-Brixlegg, Tirol)
M. Krismer, M. Tropper, P. Schneider, G. Goldenberg (Innsbruck/AT)
- P02-P04 Water proofing method for alabaster archaeological building elements by using
nano-quartz-particle coatings
M. Doukakis (Hania/GR)
- P02-P05 Plaster mortars synthesis for the consolidation of archaeological alabaster building
elements
I. Markopoulos, M. Ntoukakis (Hania/GR)
- P02-P06 Computertomographische Untersuchungen des Fettsäureangriffs auf altägyptische
Calcitalabaster-Salbgefäße
A. Franz, I. Haferkorn, K. Scholz, D. Raue, G. Kloess, K. Bente (Leipzig/DE)
- P02-P07 Geochemical characteristics of prehistoric styrian chert (silex) artefacts and their
source material
Ch. Hauzenberger, W. Postl (Graz/AT), M. Brandl (Vienna/AT), C. Kurta (Graz/AT)

- P03** **Computational and Theoretical Crystallography**
P03-P01 **Molecular structure of 4,4 di-methyl amino cyano biphenyl by X-ray diffraction and DFT calculations**
A. Chouaih, N. Benhalima, N. Boubegra, F. Hamzaoui (Mostaganem/DZ)
- P03-P02** **Molecular mechanical simulations of nitramines – a comparison of force fields**
P.B. Kempa, M. Herrmann (Pfinztal/DE)
- P03-P03** **Structure from low resolution (x-ray) powder diffraction data – slices through the Rocky Mountains of a target function**
J.M. Simons, G. Roth (Aachen/DE)
- P03-P04** **Quantumcrysca – a new approach for the prediction of molecular crystal structures by a crystallographic QM-MM-shell-model**
P. Mörschel, M.U. Schmidt (Frankfurt a.M./DE)
- P03-P05** **First principles phase diagram calculations for oxides and nitrides**
O. Adjaoud, G. Steinle-Neumann (Bayreuth/DE), B.P. Burton (Gaithersburg, MD/US)
A. van de Walle (Pasadena, CA/US)
- P03-P06** **Multifunctional oxides – influence of defects on the ferroic properties**
S. Gemming (Dresden/DE), T. Weissbach (Freiberg/DE), M. Zschornak (Dresden/DE)
H. Stöcker, D.C. Meyer (Freiberg/DE), T. Leisegang, I. Ronneberger, K. Potzger (Dresden/DE)
- P04** **Crystallography at High-Pressure-High-Temperature Conditions – from Minerals to Materials**
P04-P01 **Measurement and analysis of high-pressure pair distribution functions in diamond anvil cells at PETRA III**
N. Rademacher, W. Morgenroth, L. Bayarjargal, B. Winkler (Frankfurt a.M./DE)
- P04-P02** **First experiences with a modified 4-circle diffractometer for HP-HT single-crystal X-ray diffraction by means of laser-heating**
T. Pippinger, R. Miletich (Vienna/AT), L. Dubrovinsky (Bayreuth/DE)
- P04-P03** **Microfocus X-ray sources for high-pressure crystallography**
J. Graf, B. Hasse (Geesthacht/DE), F. Fabianni (Göttingen/DE)
M. Probert (Durham, NC/US), C. Michaelsen (Geesthacht/DE)
- P04-P04** **High-pressure phase transition of benitoite $\text{BaTiSi}_3\text{O}_9$**
C. Hejny (Innsbruck/AT), R. Miletich (Vienna/AT), A. Jasser (Heidelberg/DE)
L. Leydet (Heidelberg/DE)

- P05 Electromechanical and Optical Properties of Solids**
P05-P01 Stokes and anti-stokes lasing emission in celestine, SrSO_4 , barite, BaSO_4 and anglesite, PbSO_4
L. Bohatý, P. Becker (Cologne/DE), H. Rhee, H.-J. Eichler (Berlin/DE)
A.A. Kaminskii (Moscow/RU)
- P05-P02 Phase transition in stimulated Raman scattering (SRS)-active crystals of hardystonite, $\text{Ca}_2\text{ZnSi}_2\text{O}_7$
P. Becker, L. Bohatý, J. Liebertz (Cologne/DE), E. Libowitzky (Vienna/AT), H. Rhee
H.-J. Eichler (Berlin/DE), A.A. Kaminskii (Moscow/RU)
- P06 Environmental Mineralogy and Geochemistry**
P06-P01 will not be presented
- P06-P02 Mineralogical study of evaporite minerals in the sahl-abad playa (East of Iran)
H.A. Torshizian, H. Mollaie (Mashhad/IR)
- P06-P03 Use of an autoclave system for the study of geochemical/mineralogical rock behaviour under reservoir conditions during the geological storage of CO_2 – results of the COORALI project
M. Schmidt, H. Marbler, K. Erickson, C. Lempp, H. Poellmann (Halle, Saale/DE)
- P06-P04 Zeolite aus Porenbeton – Synthese und Eigenschaften von Wairakit und intermediärer Phase zwischen Sodalith und Cancrinit
A. Hartmann, J.-C. Buhl (Hanover/DE), Wolfgang Lutz (Berlin/DE)
- P06-P05 Heavy metal extraction from electroplating sludge using *Bacillus subtilis* and *Saccharomyces cerevisiae*
J. Wazeck (Dresden/DE)
- P06-P06 Development and assessment of water and sediment status of mining influenced watercourses – a case study at Mulde River/DE
A. Greif, W. Klemm (Freiberg/DE)
- P06-P07 On the use of an empirical model equation to predict the hydraulic conductivity of sand-kaolin mixtures
E. Steiakakis, G. Alevizos, C. Gamvroudis (Chania/GR)
- P06-P08 Radiation tolerance of potential wasteforms for plutonium disposition
G. Deissmann (Aachen/DE)

- P06-P09 **Experimental diffusion studies on water-related species through quartz**
G. Doppler, M. Baumgartner, R.J. Bakker (Leoben/AT)
- P06-P10 **As-bearing pyrite-marcasite intergrowths from the Pb-Zn Erma Reka deposit, South BG**
R. Vassileva, R. Atanassova (Sofia/BG), K. Kouzmanov (Geneva/CH)
 E. Stefanova (Sofia/BG)
- P06-P11 **The structure of schwertmannite and its relevance to ion exchange capabilities for environmental applications**
P.M. Kadletz, A.J. Götz, K. Otte, R. Pentcheva, S.-H. Park, W.W. Schmahl (Munich/DE)
 A. Ziegler (Ulm/DE), F.E. Wagner (Garching/DE), S. Pfeiffer, S. Paikaray (Bayreuth/DE)
 J. Kipry, C. Wiacek, M. Schlömann (Freiberg/DE), E. Janneck (Halsbrücke/DE)
- P06-P12 **Nitrogen in NH₄⁺-bearing illites in Carboniferous black shales – Implications for natural N₂-rich gas accumulations**
 A. Furche (Potsdam/DE)
- P07 Enzymes and Mechanisms**
- P07-P01 **Structure and function of the B-repeat from *Listeria monocytogenes* InlB**
 M. Ebbes, W. Bley Mueller, H. Niemann (Bielefeld/DE)
- P07-P02 **Crystal structure of the yeast peroxisomal α/β -hydrolase Lpx1**
H. Niemann (Bielefeld/DE), S. Thoms, J. Gärtner (Göttingen/DE)
- P07-P03 **p {margin-bottom – 0.08in} – Kinase domain of ethylene receptor activated CTR1 from *A. thaliana* is regulated through activation loop phosphorylation and dimerization**
H. Mayerhofer (Mayerhofen/AT), S. Panneerselvam, J. Müller-Dieckmann (Hamburg/DE)
- P08 Free Topics**
- P08-P01 **Mineralogy of Mg-bearing industrial minerals (Brucite-hydromagnesite) in polygenetic marble, Yazd, Iran**
 B. Taghipour (Shiraz/IR)
- P08-P02 **Production of cordierite and spinel based ceramics using bauxite, kaoline, serpentinite and dunite**
E. Thomaidis, G. Kostakis (Chania/GR)
- P08-P03 **Microstructural analyses of natural and synthesized NaCl**
 C. Tommaseo (Berlin/DE)
- P08-P04 **Oxygen ion diffusion in La_{2-x}Sr_xCuO_{4±δ} – investigated with oxygen isotope back exchange and diffraction methods**
R. Sura (Villigen/CH), M. Ceretti, C. Prestipino, W. Paulus (Rennes/FR), J. Schefer
 L. Keller (Villigen/CH), K. Conder, E. Pomjakushina (Montpellier/FR)

- P08-P05 **The dynamic three-dimensional A³B⁵ models on the example of GaAs**
K. Iskakova, R. Akhmaltdinov (Almaty/KZ)
- P09 **Functional Materials**
- P09-P01 **X-ray Diffraction and surface acoustic wave analysis of Ba_{0.65}Sr_{0.35}TiO₃ thin films**
A. Njeh (Gafsa/TN), S. Msedi (Sfax/TN), H. Fuess (Darmstadt/DE)
M. hédi Ben Ghazlen (Sfax/TN)
- P09-P02 **Structural investigations of lead-free piezoceramics**
H. Fuess, L.A. Schmitt, J. Kling, M. Hinterstein, W. Jo, S. Hayn, M. Gröting, H.-J. Kleebe
J. Rödel, K. Albe (Darmstadt/DE)
- P09-P03 **Hydrogen peroxide – a new promising solvent for the synthesis of eulytite (Bi₄(SiO₄)₃) crystals**
E. Marina, A. Marin, V. Balitsky, T. Bublikova (Chernogolovka/RU)
- P09-P04 **Phasenneubildungen und Quantifizierung von gebrannten Kalksteinen mit unterschiedlichen Calcitgehalten**
M. Riedl, E. Thorste, H. Pöllmann, T. Witzke (Halle, Saale/DE)
- P09-P05 **Microstructure development of magnesia cement during hydration**
K. Schollbach, H. Pöllmann (Halle, Saale/DE)
- P09-P06 **Growth evolution of nanosized Bi₅Ti₃FeO₁₅ by hydrothermal method along with the reaction time**
Z. Hong (Zhejiang/CN), J. Yang (Vienna/AT), T. Zhang, Y. Zhang (Zhejiang/CN)
- P09-P07 **Hierarchical growth of CdSe/Fe₃O₄ nanocomposites by solvothermal method and their growth mechanism**
J. Yang (Vienna/AT), F. Li, L. Zhou, Z. Hong (Zhejiang/CN)
- P09-P08 **New views on australian opal and opalized objects**
M. Liesegang, R. Milke (Berlin/DE)
- P09-P09 **Search for new compositions using new crystallographic data bases**
B. Kodess (Moscow/RU), P. Kodess (Aurora, CO/US)
- P09-P10 **Phase relations and thermodynamic properties of 1.13 nm tobermorite and xonotlite**
K.T. Fehr, R. Hochleitner, A. Günther (Munich/DE)
- P09-P11 **Stability relations of xonotlite-polytypes within and beyond the stability field of xonotlite**
A. Günther, K.T. Fehr, R. Hochleitner (Munich)

- P10 Inorganic Structures**
P10-P01 Crystal structure and thermochemical classification of Ba_2In
M. Bischoff, R. Niewa (Stuttgart/DE)
- P10-P02** Luminescence of divalent europium in alkaline earth metal hydrides
N. Kunkel, H. Kohlmann (Saarbrücken/DE)
- P10-P03** Gemischte Thiooxowolframate $\text{A}_2^{\text{I}}[\text{W}^{\text{VI}}\text{S}_x\text{O}_{4-x}]$
A. Lehner, C. Röhr, M. Braitsch (Freiburg/DE)
- P10-P04** Zn-Indide der Alkalimetalle mit der Anionenstruktur des β -rhomboedrischen Bors
V. Mihajlov, C. Röhr (Freiburg/DE)
- P10-P05** Zwischen Zintl, Hume-Rothery und Laves – M-reiche intermetallische Phasen
 $\text{A}^2\text{-M}^{12}\text{-M}^{12}$ ($\text{A}^2 = \text{Ca, Sr, Ba}$ / $\text{M}^{12} = \text{Zn, Cd, Hg}$)
M. Schwarz, C. Röhr (Freiburg/DE)
- P10-P06** Anomalous compression behaviour of quartz and SiO_2 -glass – a high pressure study up to 1,5 GPa
P. Mirwald, T. Loerting (Innsbruck/AT)
- P10-P07** Crystal structure analysis of layered compounds Cr_xTiS_2
K. Ohshima, S. Ikeda, T. Kawasaki, M. Takahashi (Tsukuba/JP)
- P10-P08** Investigation of structural phase transitions in letovicite $(\text{NH}_4)_3\text{H}(\text{SO}_4)_2$ at low temperatures using single-crystal X-ray and neutron diffraction
Y.J. Sohn, K. Sparta, S. Prinz (Aachen/DE), M. Meven (Garching/DE), G. Roth G. Heger (Aachen/DE)
- P10-P09** Dimorphic $\text{Ce}_4\text{N}_2\text{Se}_3$ with orthorhombic $\text{Ce}_4\text{N}_2\text{Te}_3$ - and monoclinic $\text{Nd}_4\text{N}_2\text{Se}_3$ -type structure
F. Lissner, T. Schleid (Stuttgart/DE)
- P10-P10** Synthesis and characterisation of nano- and micro-sized $\text{NaB}(\text{OH})_4$ -sodalites
C. Rüschler, A. Schulz, J.-C. Buhl (Hanover/DE)
- P10-P11** Synthesis of sodium zincophosphate sodalite influenced by sodium-polyacrylate and triethanolamine
L. Robben, J.-C. Buhl (Hanover/DE), T.M. Gelsing (Bremen/DE)
- P10-P12** Order-disorder transitions in GeTe-rich germanium antimony tellurides elucidated by in situ laue microdiffraction
P. Urban, M. Schneider, T. Schröfer (Munich/DE), X. Biquard (Grenoble/IT)
O. Oeckler (Munich/DE)

- P10-P13 **PbCa₂Al₈O₁₅ – a structure with a novel aluminate anion made up of AlO₄ tetrahedra and AlO₅ trigonal bipyramids**
M. Weil, C. Artner (Vienna/AT)
- P10-P14 **Structure elucidation of [Co(NH₃)₆][Co(CO₃)₃]**
 F. Hinrichs, A. Adam, N.-P. Pook (Clausthal-Zellerfeld/DE)
- P10-P15 **Synthesis, crystal structure and vibrational spectrum of Di-μ-aqua-bis[(nitrato)(phenanthroline)(pyridinium-4-carboxylato)-copper(II)]nitrate, [[Cu(NO₃)(INAH(phen))]₂(μ-H₂O)₂]NO₃**
 N.-P. Pook, A. Adam (Clausthal-Zellerfeld/DE)
- P10-P16 **Dimensional reduction in uranyl oxysalts with general formula A_n(UO₂)_p(TO₄)_q(H₂O)_r (A = monovalent cation, T = S, Se, Cr, Mo)**
V. Kovrugin, V. Gurzhiy, S. Krivovichev (St. Petersburg/RU), I. Tananaev (Moscow/RU)
- P10-P17 **Isomorphous transition metal substitution in PbAlBO₄**
M.M. Murshed, A. Rusen, R. Fischer, T. Gesing (Bremen/DE)
- P10-P18 **Boron mullites**
H. Lührs, R. Fischer, H. Schneider (Bremen/DE)
- P10-P19 **Synthese und Kristallstruktur des Nickel(II)-Dodekahydroxo-closo-Dodekaborat-Hydrats [Ni(H₂O)₆][B₁₂(OH)₁₂]**
L.W. Zimmermann, T. Schleid (Stuttgart/DE)
- P10-P20 **Ein Lithium-Natrium-Aluminium-Oxophosphat der Zusammensetzung Li₈NaAl₃[PO₄]₂[P₂O₇]₃ mit Na⁺-leitenden Kanälen**
S.J. Metzger, T. Schleid (Stuttgart/DE)
- P10-P21 **Single crystals of BaY₂Se₄ with CaFe₂O₄-type structure**
 C. Schurz, C.F. Kuhn, T. Schleid (Stuttgart/DE)
- P10-P22 **New orthomolybdates in the Cs-Fe(II,III)-Mo-O system – Cs₄Fe(MoO₄)₃, Cs₂Fe₂(MoO₄)₃ and CsFe₅(MoO₄)₇**
A. Sarapulova, T. Namsaraeva, D. Mikhailiva (Dresden/DE, Ulan-Ude/RU)
 N. Kuratieva (Novosibirsk/RU), A. Senyshyn (Munich/DE), H. Ehrenberg (Dresden/DE)
 B. Bazarov (Ulan-Ude/RU)
- P10-P23 **A novel crystal structure type shown by a flux-grown tetragonal Ba-Y-silicate and its isotypic Ho-analogue**
M. Wierzbicka-Wieczorek (Jena/DE), U. Kolitsch, E. Tillmanns (Vienna/AT)

- P10-P24 **Synthesis and crystal structure of $\text{Li}_2\text{H}_2\text{P}_2\text{O}_6 \cdot 2\text{H}_2\text{O}$**
P. Wu, M. Gjikaj (Clausthal-Zellerfeld/DE)
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Maney Publishing (Leeds/GB)

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Springer Science + Business Media B.V. (Dordrecht/NL)

"Biogeochemistry"

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DGK 2012

100 Years of X-Ray Diffraction

Laue Day and 20th Annual Meeting of the
German Crystallographic Society (DGK)



12–15 March 2012

MUNICH

An international conference commemorating the discovery of X-Ray diffraction by Max von Laue, Walter Friedrich and Paul Knipping at LMU Munich in 1912

www.dgk-conference.de

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Guided Tour through Salzburg “The Classic”

Join our certified tour guide on a classic old town walk and discover what Salzburg has to offer. Did you know that Mozart was a regular guest at Tomaselli, Salzburg’s oldest coffee house, drinking almond milk? Or have you always wanted to explore “the Rome north of the Alps” and marvel at the masterly architecture?

Passing Mozart’s birthplace you will walk towards baroque Salzburg, which has been the seat of archbishops and sovereigns for more than 1,000 years and has been declared World Heritage Site by the UNESCO in 1997. All of this and much more will your guide tell you, show you, and explain to you in lively pictures in a two-hour tour.



Source: Tourismus Salzburg

Date	Tuesday, 20 September 2011
Time	14 ⁰⁰
Duration	2 h
Fee	7 EUR
Meeting point	Check-In, 14 ⁰⁰ (tour ends in the city centre at “Mozartplatz”)

Get-Together

Come together for drinks and snacks prior to the kick-off of the conference and break the ice in first conversations with our industrial partners and your colleagues.

Date	Tuesday, 20 September 2011
Time	19 ¹⁵
Fee	included



Source: fotolia.com/Tim Porter

Registration required!

Guided Tour of the history of beer in Salzburg

If you always wanted to know, why exactly Salzburg has such a diverse and special beer culture and you want to find what the historical background of that is, then you’ll have a pleasant time during this tour.

On this trip you’ll not just find out where the “Stieglbrewery” got it’s name from and why the abbey Mülln is such a magnet for beer lovers, furthermore you’ll discover the mystery of the “water equestrian of the Untersberg” and find out which beer Mozart liked the most.



Source: Tourismus Salzburg

Date	Wednesday, 21 September 2011
Time	14 ⁰⁰
Duration	3 h
Fee	13 EUR
Meeting point	In front of the main entrance of the conference venue at “Hellbrunner Straße”, 14 ⁰⁰

Social and Cultural Programme

City Walk Salzburg "Hidden Treasures"

This guided tour will show you hidden, barely visible and many things which can easily be missed at first sight. Take a walk through Salzburg and enjoy beautiful and funny details of the city.

Date	Thursday, 22 September 2011
Time	14 ⁰⁰
Duration	3 h
Fee	8 EUR
Meeting point	Check-In, 13 ⁴⁵ (tour ends in the city centre at "Mozartplatz")



Source: Tourismus Salzburg

Social Evening "StieglKeller"

The highlight of Salzburg hospitality and beer garden culture shines far over the roofs of the old town. Lying under the protection of the mighty Hohensalzburg Fortress, you can delight in a magnificent view. The wonderful snugs are full of spaciousness and at the same time cosiness.

Date	Thursday, 22 September 2011
Start	20 ⁰⁰
Fee	30 EUR
Address	Restaurant StieglKeller Festungsgasse 10* 5020 Salzburg



Source: Zentrale IMLAUER
Hotels & Restaurants

* please note, that you should use the parking garage "Altstadtgaragen". There are no parking possibilities next to the restaurant. Bus lines 3 and 8 stop nearby the "Mozartplatz". From there it is just a 5-10 minute walk to the "StieglKeller".

Guided Tour fortress Hohensalzburg

Fortress Hohensalzburg is a monument of over 900 years and is one of the largest existing 11th century fortresses in Europe. Every crevice of the walls, every nook and cranny of this magnificent complex brings forth its own fascinating background information, stories, myths and legends.

Date	Friday, 23 September 2011
Time	14 ⁰⁰
Fee	15 EUR
Meeting point	Check-In, 13 ⁰⁰



Source: Tourismus Salzburg

Orchestra concert

The Mozart Orchestra Salzburg, a traditional chamber orchestra, was founded to perform the enchanting masterpieces of the great artists of music – mainly the works of W.A. Mozart.

Extract of the programme:

W.A. Mozart:

Concert for piano and strings

Salzburg Symphonies

Concert for Horn and strings

Concert for Alphorn and strings

"A little night music" etc.



Source: Camerata Salzburg

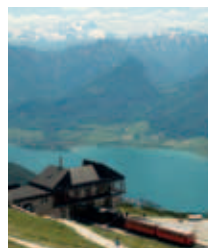
Date Friday, 23 September 2011
Time 20⁰⁰
Address: Festung Hohensalzburg
"Goldener Saal"
Mönchsberg 34*
5020 Salzburg

* please note, that you should use the parking garage "Altstadtgaragen". There are no parking possibilities at the mountain. You can use the mountain railway "Festungsbahn" which starts at the "Festungsgasse" and ends at the "Hohensalzburg" at the mountain. The mountain railway just serves until 20⁰⁰. Of course you can walk via "Festungsgasse" at the top. Bus lines 3 and 8 stop nearby the "Mozartplatz". From there it is just a 5-10 minute walk to the "Festungsgasse".

Registration Deadline: 20 August 2011

Conference Excursion and Boat Cruise Wolfgangsee

We would like to invite you to join our conference excursion to one of the most beautiful destinations in the Salzkammergut region – Wolfgangsee and Schafberg. The journey will start at the main train station of Salzburg. A bus will bring you to the beautiful St. Gilgen. From here you will join a boat cruise on the famous Wolfgangsee. When you reached St. Wolfgang, you will experience the exciting drive with the Schafbergbahn, which will bring you to top of the mountain. The drive with that railway will make your journey to an unforgettable experience. At the top of the Schafberg, you will enjoy impressive Alpine views in multiple directions. At the Hotel Schafbergspitze, Austria's oldest mountain inn, you will be provided with a traditional Austrian meal. Estimated arrival time in Salzburg is 18⁰⁰.



Source: www.schafbergbahn.at

Date Saturday, 24 September 2011
Time 8⁰⁰
Duration 10 h
Fee 60 EUR
Meeting point Salzburg Main Station, Südtiroler Platz

General Information

Arrival by car/Parking

The Department of Materials Engineering and Physics of the University of Salzburg and the city centre are linked to both the motorways A1 and A10 as well as to the federal roads B150 and B155.

Address for GPS navigation systems: Hellbrunnerstraße 34, (crossroad "Michael-Pacher-Straße", please drive via "Alpenstraße") 5020 Salzburg (Austria).

The Department of Materials Engineering and Physics offers payable parking in basements inside of the complex. A limited capacity of parking space will be reserved and marked. Access will be limited and please note further details currently on the conference homepage. There is also a large car park on the Makartplatz, which is about 2 km away from the venue.

P+R Parking Salzburg Süd

Public transportation by bus in Salzburg

The main train and bus station are connected with bus routes 3 and 8, which travel frequently and directly to the main station and city centre. Make sure to use bus stop „Faistauergasse“ on „Alpenstraße“. From there it is a 5 to 10 minute walk to go to the venue in "Hellbrunnerstraße" via "Faistauergasse", "Mascagnigasse" and "Michael-Pacher-Straße" to the venue in "Hellbrunnerstraße".

The bus route 22 serves the stop "Bocksbergerstraße", which is 60m away from the venue. This line drives more infrequently, you have to change busses and drive longer. Therefore we would recommend to take lines 3 and 8.

Certificate of Attendance

Certificates of attendance will be distributed at the check-in.

Evaluation

Please turn in your completed and legible evaluation form to the info desk or check-in on the last day. We are always striving to provide high congress quality. This goal can only be reached with your help, your active participation and constructive criticism.

Opening Hours

	Tuesday	Wednesday	Thursday	Friday
Industrial Exhibition	18 ⁰⁰ –21 ⁰⁰	10 ⁰⁰ –16 ⁰⁰	10 ⁰⁰ –16 ⁰⁰	10 ³⁰ –13 ⁰⁰
Poster Exhibition	---	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –19 ⁰⁰	08 ⁰⁰ –11 ³⁰
Check-In	14 ⁰⁰ –21 ⁰⁰	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –19 ⁰⁰	08 ⁰⁰ –13 ⁰⁰
Media Check-In	14 ⁰⁰ –21 ⁰⁰	08 ⁰⁰ –18 ⁰⁰	08 ⁰⁰ –19 ⁰⁰	08 ⁰⁰ –11 ³⁰

Internet

There are computers with internet access available at the media check-in. If you would like to browse with your own notebook, you can use the WLAN.

WLAN Access Data

Network name: Joint Meeting 2011 User name: attendee Password: salzburg

Publishing of Abstracts

Printed versions will be handled out for free to all DGK Members who attend the conference.

If you are not a member of the DGK, you can order a printed version for 20 Euro. For further information and your order please refer to www.salzburg2011.org or please ask at the check-in.

City Plan



Source: Salzburg Information

General Hints for Authors and Presenters

Presentation Submission

Media check-in is situated on the ground floor next to the plenary hall.

Time Allocation

We ask you to please follow the following. Please prepare your presentation so that you remain within the time allotment. Chair persons (Convener) been advised to avoid delays. Contact your chair person before your session begins and advise of any changes or special wishes.

Presentation Form/Submission of Presentation

PDF and PowerPoint presentations are permitted.

Open Office formats may also be used. Required technical equipment will be available at the congress.

The use of Macintosh or Open Office formats as well as the use of a personal laptop for a presentation is not planned, but possible.

For video and audio files please submit AVI, WMV and MPG files only as a separate file.

Please make sure that any required CODEC files for any videos are also submitted.

Your presentation and any additional files should be submitted at least two hours before your presentation time.

Please note: If you use a USB stick to save your files, do not protect it with software.

The projection data of your presentations before and during the whole congress will be recorded and managed centrally. There is a notebook with MS PowerPoint 2007 and a video projector in location.

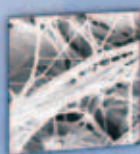
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Die Zeitschrift

In den *Nachrichten aus der Chemie* machen Wissenschaftler auf das hohe Potenzial ihrer Forschungsergebnisse aufmerksam, denn Spitzenforschung ist zu wertvoll, um nach jahrelanger intensiver Arbeit nur in Primärjournalen publiziert zu werden.

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General Terms and Conditions

Registration and Confirmation

Registration is subject to capacity limitations. Registration must include the name of any accompanying person to ensure their inclusion into the planning of the social programme. Upon receipt of registration invoice or confirmation, registration is considered official and effectual. This document is a valid VAT invoice which may be submitted to the local tax and revenue office for tax purposes.

Invoicing and Due Date for Fees

Fees for the scientific programme, the social evening and the social programme of the event will be charged in the name and on behalf of Conventus GmbH inclusive the statutory VAT rate of 20% (Austrian Taxes). All fees are due upon receipt of the registration invoice or confirmation form. Transfer payments must include the name of the participant and the invoice number, otherwise they will not be accepted. All major credit cards are accepted.

Scope of Services

Event fees include participation in the scientific programme only. Additional fees for the social programme will apply. Included in this fee are programme book, abstract CD, name tags and a certificate of attendance. These items are generally handed out at the venue.

Cancellations, Changes, Refunds

Cancellations can be made in written form only and will only be accepted if received by 9 August, 2011. A cancellation fee of 25 EUR will apply. The same terms apply for cancellations of the social programme, however no cancellation fee will be charged. Any cancellations after this date or no-shows at the event are not eligible for a refund and the full fee in accordance to the registration invoice or confirmation will be due. Any changes in booking, after booking confirmation has been issued, will result in a handling fee of 15 EUR. Any requested additions to existing reservations or reservations made during the event on-site will be processed according to availability.

Event Cancellation, Refunds

There is limited capacity for all events. For certain events a minimum number of participants is required. If the minimum number of participants is not reached, the organiser reserves the right to cancel all or parts of the event on a short-term notice. In this case, all paid fees will be fully refunded.

Force Majeure, Disclaimer

The organiser is responsible for all changes to individual parts of the event. Claims for damages are excluded if the staging of the event or individual components are hampered or prevented by unexpected political or economic events or generally by force majeure or by the cancellation of speakers or if similar changes are required.

Hotel Reservations, Disclaimer

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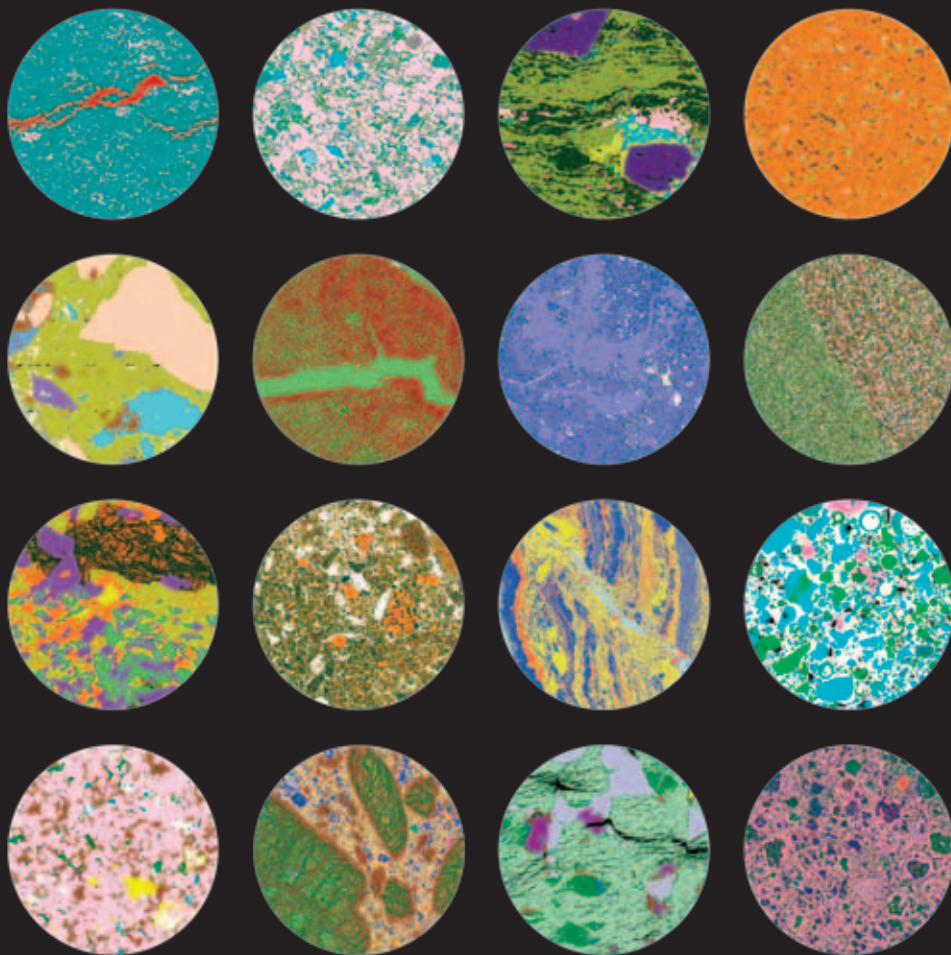
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