

ECMS 2011

7th European Conference on
Mineralogy and Spectroscopy

Program

September 4th - 7th 2011
Potsdam, Germany

Monday September 5 – Morning Session

9.15 – 9.30 *Opening*

Session Chair: Khomenko V. M.

9.30 – 10.15 *Key Note Talk*

Hofmeister A. M.

Understanding Heat Transfer from the Perspective of IR to UV Spectroscopy

10.15 – 10.30 *Thomas S.-M., Jacobsen S. D., Bina C. R., Goncharov A. F., Frost D. J. & McCammon C. A.*

Temperature- and pressure-dependent radiative thermal conductivity of transition zone minerals – Implications for the Earth's interior

10.30 – 10.45 *Bolfan-Casanova N., Muñoz M., McCammon C., Deloule E., Férot A., Demouchy S., France L., Andrault D. & Pascarelli S.*

Ferric iron and water incorporation in wadsleyite under hydrous and oxidizing conditions: a XANES and SIMS study

10.45 – 11.00 *Mrosko M., Lenz S., McCammon C. A., Taran M., Wirth R. & Koch-Müller M.*

Incorporation of Fe³⁺ in ringwoodite studied via EELS, FTIR-, and Mössbauer spectroscopy

11.00 – 11.30 *Coffee Break*

Session Chair: Thomas S.-M.

11.30 – 11.45 *Jahn S., Wunder B., Koch-Müller M., Watenphul A. & Taran M. N.*

Spectroscopic, structural and computational study of guyanaite, β -CrOOH

11.45 – 12.00 *Khomenko V. M., Wirth R. & Gottschalk M.*

OH species on Crystal-Glass border in LAS Glass-Ceramics

12.00 – 12.15 *Dulski M., Kusz J., Wrzalik R., Hawelek L., Bilewska K., Szade J. & Galuskin E. V.*

Reasons for reduction of perfect symmetry on the example of rondorfite

12.15 – 12.30 *Hansen A.-L., Mihailova B., Peters L. & Depmeier W.*

Raman Spectroscopic Investigations of Aluminate Sodalites

12.30 – 12.45 *Lazor P., Hålenius U., Skogby H. & Bosi F.*

Raman spectroscopic study of structural relaxation and cation occupancies in a spinel solid solution

13.00 – 14.15 *Lunch Break*

Monday September 5 – Afternoon Session

Session Chair: Marquardt H.

- 14.15 – 15.00 *Key Note Talk*
Speziale S., Marquardt H. & Reichmann H. J.
Elastic properties of materials by Brillouin Scattering
- 15.00 – 15.15 Laukamp C., Termin K. A., Cudahy T. & Haest M.
Vibrational Spectroscopy of Calcic Amphiboles - From Mineral Physicochemistry to Applications in Mineral Exploration
- 15.15 – 15.30 Watenphul A. & Schmidt C.
Insight into structural changes in berlinite (AlPO₄) from in-situ Raman spectroscopy at high pressure and temperature
- 15.30 – 15.45 Spiekermann G., Steele-MacInnis M., Schmidt C. & Jahn S.
Mode-projected vibrational analysis and Raman spectra of silica species in aqueous solution using ab initio molecular dynamics
- 15.45 – 16.15 *Coffee Break*
- 16.15 – 17.30 **Poster Session: Discussion of Posters P1 – P20**
(All Posters are displayed all three days)
- P1 Bailau R., Galuskin E. V., Gazeev V. M. & Galuskina I. O.
Raman investigation of potential new mineral - Fe³⁺-analogue of wadalite from calcareous-silicate xenoliths of the Upper Chegem caldera, Northern Caucasus, Russia
- P2 Banasik K.
Raman investigation of Ca₅(SiO₄)_{1.5}(SO₄)_{1.5}(OH,F) - Ca₅(AsO₄)₃(OH,F) - Ca₅(PO₄)₃(OH,F) series from calc-silicate xenoliths of the Upper Chegem caldera, Northern Caucasus, Russia
- P3 Bobocioiu E. & Caracas R.
Theoretical Raman spectra of carbonate minerals
- P4 Dobretsova E., Kurazhkovskaya V., Borovikova E. & Boldyrev K.
Vibrational spectra and the crystal growth of huntite-like chromium borates RCr₃(BO₃)₄, where R = La – Er
- P5 Dumitras D.-G., Marincea S., Bilal E. & Constantinescu E.
Infrared spectroscopy of ardealite from the “type locality” Cioclovina Uscata Cave, Sureanu Mountains, Romania
- P6 Hinrichs R. & Vasconcellos M. A. Z.
Chlorapatite identification in Putinga meteorite using Raman spectroscopy
- P7 Isaenko S., Shumilova T. & Mayer J.
Raman spectroscopy of lonsdaleite and diamond from Kumdykol deposit (Kazakhstan)
- P9 Kristova P., Hopkinson L. & Rutt K.
FT-Raman quantitative analyses of multi-minerallic carbonate bearing powders

Monday September 5 – Afternoon Session

- P10 Libowitzky E., Bechtold A., Friesl P., Oberwandling L. & Wildner M.
Influence of surface defects on Raman spectra of ore minerals
- P11 Makreski P., Jovanovski S., Pejov L., Kloess G., Hoebler H.-J. & Jovanovski G.
Theoretical and Experimental Study of the Vibrational Spectra of Sarkinite $[\text{Mn}^{2+}_2(\text{AsO}_4)(\text{OH})]$ and Adamite $[\text{Zn}_2(\text{AsO}_4)\text{OH}]$
- P12 Salama W., Ciobota V., El Aref M. & Gaupp R.
Identification of the mineralogy and organic materials of the Cretaceous and Middle Eocene ironstones by means of FTIR and micro-Raman spectroscopy
- P13 Seaman S., Williams M. & Koteas C.
The Effects of Water in Nominally Anhydrous Minerals on Anatexis of Lower Crustal Granitoids
- P14 Skogby H., Lazor P. & Bosi F.
Local arrangement around OH groups in tourmaline studied by vibrational spectroscopy and structural refinement
- P15 Waesermann N., Schlüter J., Bergemann C., Bersani D. & Mihailova B.
Raman spectroscopy on garnet and ruby as a non-destructive analytical method in gemmology
- P16 Schmidt C., Steele-MacInnis M. & Wilke M.
Raman spectroscopic study of zircon to high pressure and temperature
- P17 Koch-Müller M., Mrosko M., Gottschalk M. & Schade U.
Pressure-induced phase transitions in Ilvaite: a Mid/Far Micro-FTIR spectroscopic study
- P18 Lucassen F., Koch-Müller M., Taran M. & Franz G.
Hydrogen incorporation into pure and Nb-, Cr-, V-doped synthetic rutile at 600°C, 400MPa
- P19 Marquardt H., Marquardt K. & Speziale S.
Focused Ion Beam preparation and characterization of single-crystal samples for high-pressure experiments in the diamond-anvil cell
- P20 Eisele A., Chabrilat S., Lau I., Wheaton B., Carter D., Ong C., Hewson R., Cudahy T. & Kaufmann H.
Use of VNIR-SWIR and TIR diffuse reflectance spectroscopy for the quantitative prediction of common soil properties

Tuesday September 6 – Morning Session

Session Chair: Lazor P.

- 9.00 – 9.45 *Key Note Talk*
Antonangeli D.
Elasticity of Earth's deep interior probed by Inelastic X-ray Scattering
- 9.45 – 10.00 Giuli G., Cicconi M. R. & Paris E.
^[4]Fe³⁺-O distance in synthetic kimzeyite garnet
- 10.00 – 10.15 Bordage A., Rossano S. & Fuchs Y.
X-ray Natural Linear Dichroism: The case of alexandrite BeAl₂O₄:Cr³⁺
- 10.15 – 10.30 Di Benedetto F., Capacci F., D'Acapito F., Fornaciai G., Innocenti M., Montegrossi G. & Romanelli M.
Fe speciation in industrial quartz reagents: insights from XAS spectroscopy on bulk materials and suspended dusts
- 10.30 – 10.45 Shiryaev A., Zubavichus Y., Burakov B. & Kalmykov S.
XAFS of Pu-doped zircon and monazite: Pu and U environment
- 10.45 – 11.00 Simon S., Wilke M., Caliebe W. & Kvashnina K.
RIXS and XANES spectroscopy study of La bearing compounds and La-doped silicate glasses
- 11.00 – 11.30 *Coffee Break*

Session Chair: Rossano S.

- 11.30 – 11.45 Dubrail J., Jahn S., Wilke M. & Schmidt C.
Complexation of high-field strength elements in subduction zone aqueous fluids: Ab initio molecular dynamics and X-Ray absorption spectroscopy
- 11.45 – 12.00 Sternemann C., Mende K., Nyrow A., Sahle C. J., Wilke M., Schmidt C., Simonelli L., Moretti Sala M. & Tolan M.
X-ray Raman scattering: A spectroscopic tool for in-situ studies of low Z element's absorption edges at high pressure and high temperature
- 12.00 – 12.15 Taylor R. P., Mosselmans J. F. W., Finch A. A. & Quinn P. D.
Time Resolved Fluorescence of Framework Silicates
- 12.15 – 12.30 Salge T., Tunckan O., Turan S., Kearsley A. & Terborg R.
From the micro- to nanoscale: How far can peak deconvolution be taken using Energy Dispersive X-ray Spectroscopy (EDS) with SEM?
- 12.30 – 12.45 Appel K., Appel P., Möller A. & Martinez-Criado G.
Elemental nano-imaging and chemical U-Th-Pb dating of monazite and zircon using synchrotron radiation induced XRF
- 13.00 – 14.15 *Lunch Break*

Tuesday September 6 – Afternoon Session

Session Chair: Jahn S.

- 14.15 – 15.00 *Key Note Talk*
Wentzcovitch R.
Spin States in the Earth's Mantle
- 15.00 – 15.15 Caracas R.
Spin transition in Fe-bearing perovskite: implications for the lower mantle
- 15.15 – 15.30 Shchapova Y., Votyakov S., Kuznetsov M. & Ivanovskii A.
X-ray emission and X-ray photoelectron spectroscopy studies, ab initio electronic structure calculations of radiation damaged zircon and monazite
- 15.30 – 15.45 Fechtelkord M., Langner R., Garcia A., Palin E. J. & López-Solano J.
Aluminum ordering and clustering in Al-rich synthetic phlogopite:
{¹H} → ²⁹Si CPMAS HETCOR spectroscopy and atomistic calculations
- 15.45 – 16.15 *Coffee Break*
- 16.15 – 17.30 **Poster Session: Discussion of Posters P21 – P33**
(All Posters are displayed all three days)
- P21 Goettlicher J. & Steininger R.
K-edge XANES Spectroscopy on sulfur and phosphor in silicate minerals
- P22 Di Benedetto F., D'Acapito F., Innocenti M., Lavacchi A., Montegrossi G., Pardi L. A. & Romanelli M.
Preliminary X-ray Absorption Spectroscopy study of synthetic nanokuramite
Cu₃SnS₄
- P23 Rossano S., Trcera N., van Hullebusch E., Jean-Soro L., Bordage A., Berger P. & Labanowski J.
Bioweathering of Mg-bearing silicate glasses in presence of heterotrophic bacteria
- P23x Ferrand J., Rossano S., Loisel C., van Hullebusch E., Trcera N., Farges F., Oriol G., Bousta F. & Pallot-Frossard I.
The browning phenomenon of medieval stained glass windows.
- P24 Borchert M., Wilke M. & Appel K.
Eu³⁺/Eu²⁺ ratios in glass equilibrated with plagioclase by micro XANES
- P25 Cicconi M. R., Giuli G., Paris E., Ertel-Ingrisch W., Dingwell D. B. & Ulmer P.
Structural behaviour of europium in silicate glasses
- P26 Trcera N., Rossano S. & Cabaret D.
Contribution of Molecular Dynamics simulations and ab initio calculations to the interpretation of Mg K-edge experimental XANES in silicate glasses
- P27 Wilke M., Machek P. & Caliebe W. A.
Non-resonant and resonant X-ray Emission spectroscopy on iron-bearing minerals and glasses
- P28 Nyrow A., Mende K., Sahle C. J., Schmidt C., Sternemann C., Wilke M., Simonelli L., Moretti Sala M., Hiraoka N., Wieland D. C. F., Gordon A. R., Tolan M. & Tse J. S.
Study of silicate melts and iron oxides by x-ray Raman scattering
- P29 Sahle C. J., Schmidt C., Sternemann C., Wilke M., Simonelli L., Nyrow A., Mende K. & Tolan M.
Structural changes of water at high pressure and high temperature: information from X-ray Raman scattering at the oxygen K-edge

Tuesday September 6 – Afternoon Session

- P30 Romanelli M., Di Benedetto F., D'Acapito F., Innocenti M., Fornaciai G., Zoleo A., Bartali L. & Capacci F.
Insights to crystal chemistry of defects during industrial processing from ESEEM spectroscopy
- P31 Romanelli M., Innocenti M., De Luca A., Bencistà I., Di Benedetto F., Lavacchi A., Pardi L. A. & Foresti M. L.
New technologic Substrates by Electrodeposition for Energy devices: an XPS study of Cu- and Sn- sulfides
- P32 Lastusaari M., Bettinelli M., Eskola K. O., Hölsä J., Jungner H., Kotlov A., Laamanen T., Malkamäki M. & Welter E.
The Bologna Stone: History's First Persistent Luminescent Material
- P33 Bobocioiu E. & Caracas R.
Complexity in low-temperature phase diagrams of planetary ices: phase transition in bischofite, $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$

Wednesday September 7 – Morning Session

Session Chair: Lottermoser W.

- 9.00 – 9.45 *Key Note Talk*
Taran M.
Optical absorption spectroscopy of transition metal ions-bearing minerals at different temperatures and pressures: some crystal chemical and thermodynamic aspects
- 9.45 – 10.00 Andreozzi G. B., D'Ippolito V., Bosi F. & Halenius U.
Structural relaxation around Co^{2+} in synthetic blue $(\text{Mg},\text{Co})\text{Al}_2\text{O}_4$ spinel crystals
- 10.00 – 10.15 Zherebetsky D., Lebernegg S., Amthauer G. & Grodzicki M.
Magnetic structure of almandine
- 10.15 – 10.30 Dainyak L. G., Rusakov V. S., Sukhorukov I. A. & Drits V. A.
Reconstruction of octahedral cation distribution in 2:1 phyllosilicates and interpretation of their Mössbauer spectra
- 10.30 – 10.45 Petrova E., Oshtrakh M., Grokhovsky V. & Semionkin V.
Comparative Study of Olivine in Pallasites and Chondrites Using Mössbauer Spectroscopy with a High Velocity Resolution
- 10.45 – 11.00 Filip J., Bosi F., Novák M., Skogby H. & Wildner M.
The role of iron in Fe-rich tourmaline: results of high-temperature experiments
- 11.00 – 11.30 *Coffee Break*

Session Chair: Fechtelkord M.

- 11.30 – 11.45 Rüscher C. H., Steinke H. & Wiencke J.
Temperature dependent absorption spectra of biotites and olivines reinvestigated: on the distinction of polaron and exciton excitations
- 11.45 – 12.00 Russina M. & Kemner E.
Microscopic Behavior of Gas Clathrates Studied by cold Time-of-Flight Neutron Spectroscopy
- 12.00 – 12.15 Montegrossi G., Di Benedetto F., Pardi L. A. & Romanelli M.
Characterization of temperature behaviour of Mn^{2+} in calcite by electron paramagnetic resonance (EPR)
- 12.15 – 12.30 Caracas R. & Bobocioiu E.
The WURM project - a freely available web-based repository of computed physical data for minerals
- 12.30 – 12.45 Wathanakul P., Monarumit N., Leelawatanasuk T., Ingavanija S., Sriprasert B. & Atichat W.
A Contribution to Indicating the Low Temperature Heat Treatment of Ruby Samples from Myanmar and Vietnam
- 13.00 – 14.15 *Lunch Break*

Wednesday September 7 – Afternoon Session

Session Chair: Appel K.

- 14.15 – 15.00 *Key Note Talk*
Farges F.
The French Blue diamond : how spectroscopy reveals an unsuspected masterpiece
- 15.00 – 15.15 Waesermann N., Mihailova B., Gospodinov M. & Bismayer U.
In-situ high-pressure and high-temperature Raman spectroscopy on advanced perovskite-type relaxor ferroelectrics
- 15.15 – 15.30 Shi J., Bismayer U. & Becker K.-D.
Optical Absorption Spectroscopy of Local Structure and Kinetic Processes in Minerals
- 15.30 – 15.45 Borovikova E. & Kurazhkovskaya V.
Vibrational spectroscopy of mineral-like functional materials with complex crystal structures
- 15.45 – 16.15 *Coffee Break*
- 16.15 – 17.30 **Poster Session: Discussion of Posters P34 – P53**
(All Posters are displayed all three days)
- P34 Ollier N., Fuchs Y., Rossano S., Bordage A., Leal J. M. & Horn A. H.
Cr³⁺ optical properties of Brazilian beryl and chrysoberyl (alexandrite and emerald)
- P35 Talla D., Wildner M. & Beran A.
Polarised absorption spectra of wulfenite in the OH vibrational and UV-Vis spectral regions
- P36 Wala T., Psiuk B., Kubacki J. & Stec K.
Spectroscopic study of andalusite originating from both autochthonous and eluvial deposits
- P37 Tomašić N., Bermanec V., Plodinec M. & Gajović A.
Samarskite high-temperature modification recrystallisation: vibrational spectroscopy probing
- P38 Todoran R., Todoran D. & Vida-Ratiu A.
UV-VIS reflective spectroscopy measurement of optical functions and of certain energy characteristics specific to sulphurous minerals (Sphalerite, Galena, Chalcopyrite)
- P39 Petrovsky V. A., Vasilyev E. A., Lutoev V. P., Silaev V. I., Kozlov A. V., Sukharev A. E. & Martins M.
Spectroscopy of the brazilian diamonds
- P40 Sukharev A. E., Glukhov Y. V., Isaenko S. I. & Khityunin V. P.
Similarities some spectroscopic characteristics of placer diamonds and carbonado brazil
- P41 Lorek A., Wagner N. & deVera J. P. P.
Estimation of ice and liquid water content of two martian analogue soils in a temperature range from 0 °C to -70 °C by means of dielectric spectroscopy
- P42 Lottermoser W., Weber S.-U., Grodzicki M., Redhammer G., Tippelt G., Litterst F., Dlugosz S., Becker K.-D., Bank H. & Amthauer G.
The Electric Field Gradient In Natural Chrysoberyl And Sinhalite

Wednesday September 7 – Afternoon Session

- P43 Lottermoser W., Weber S.-U. & Kirfel A.
The Electric Field Gradient In Synthetic Fayalite (A Supplement)
- P44 Aparicio C., Filip J., Marusak Z. & Mashlan M.
Mechanism of reductive decomposition of $\text{Fe}_{1-x}\text{Mg}_x\text{Al}_2\text{Si}_3\text{O}_{12}$ garnets: The crucial role of iron content
- P45 Maheswaramma K. S., Reddy S. L. & Reddy A. V.
EPR and Optical absorption spectral studies on sphalerite mineral
- P46 Abd El Rahim S. H., El Nashar E. S. R., Osman A. F. & Abd El Ghaffar N. I.
Gold-bearing sulphides associated with the granitic wall rock alterations at the Fawakhir area, Central Eastern Desert, Egypt
- P47 Sokolov S., Chistyakova N., Orlova N. & Shuvalova Y.
The first discovery of donnayite-(Y) in a gold deposit
- P48 Călin N., Dumitraş D.-G., Marincea Ş., Iancu A. M., Ghineţ C. & Anason A. M.
Pegmatite phosphates, Coşu field, Cibin Mountains, Romania
- P49 Mashukov A. & Mashukova A.
The structural properties of Norilsk type ores
- P50 Melegy A.
Distribution and speciation of heavy metals in El Fayoum soil, Egypt
- P52 Sadek Ghabrial D.
Biotite - chlorite transformation during low temperature alteration
- P53 Sarrafi M.H., Youzbashi A.A., Ahmadi K. & Bahrevar M.A.
Marble deterioration in Chaharbagh school in Isfahan by atmospheric pollutants