

NCS2014 Program at a glance

THURSDAY	FRIDAY	SATURDAY
25 September	26 September	27 September
Registration 8:00-16:30	-	-
Opening ceremony 9:00-9:30	Plenary Lecture (in Bulgarian) Prof. Georgi Kirov	Session VII 9:00-10:20
Session I 9:30-10:30 J. Manuel Perez-Mato (I) Vesselin Tonchev (OP)	Session V 9:50-10:30 Jörg Rothe (I)	Emre S. Tasci (I) Thomas Kerestedjian (PO) D. Nihtianova (PO)
Coffee break & NCS14 Photo	Coffee break	Coffee break
Session II 11:00-12:30 Ross Angel (I) Milen Gateshki (OP) Boris Shivachev (OP)	Session V (continued) 11:00-12:20 Tonya Vitova (I) B. Mihailova (OP) Victor Ivanov (OP)	Session IX 10:50-12:10 Rossitza Pentcheva(I) Zara Cherkezova-Zheleva (OP) G. Avdeev (OP)
Lunch break	Lunch break	Closing remarks & Award for the best poster contribution by young scientists Rositsa Nikolova President of BCS 12:10 – 13:00
Session III 13:40-15:00 Ulrich Bismayer (I) Rossitsa. Titorenkova (OP) Tzanko. Doukov (OP)	Session VI 13:40-16:10 Biliana Gasharova (I) V. Karadjova (OP) Krassimir Garbev (I) Al. Karamanov (OP) Alaa Adam (OP) Aquachim (IT)	
Session IV 15:00-16:40 Maria Lalia-Kantouri (I) G. Gencheva (OP) L. Tzvetanova/T.Todorova (OP) Bas ter Mull, PANalytical (IT) Rofa/Rigaku (IT)		
Poster Session (snacks & drinks) Presenting <u>Odd</u> PS numbers 16:40-19:00	Poster Session (snacks & drinks) Presenting <u>Even</u> PS numbers 16:50-19:00	
Annual meeting of the Bulgarian Crystallographic Society 19:00-19:30		Legend: PL: Plenary Lecture, I: Invited Speaker, OP: Oral presentation, IT: Industrial talk PS: Poster session

SYMPOSIUM PROGRAM

Thursday 25 September

8:00 **Registration**

9:00–9:30 **Opening ceremony**

Chairing: Irena Mihaylova

Welcome address from **Mitko Georgiev**,
Rector of the University of Chemical Technology and Metallurgy

Introductory remarks by **Mois Aroyo**
Universidad del Pais Vasco, Bilbao, Spain

Welcome address by **Dr. Todor Chobanov**, deputy mayor of Sofia

Welcome musical performance

Session I **Chairing: Rositsa Nikolova**

9:30–10:10 **J. Manuel Perez-Mato* (invited)**, B. Kocsis, E. Tasci, M. Aroyo
** Dept. de Fisica de la Materia Condensada, Facultad de Ciencia y
Tecnologia, Universidad del Pais Vasco (UPV-EHU), Bilbao, Spain*
Single mode signature in distorted phases revealed by symmetry-mode analysis

10:10–10:30 **Vesselin Tonchev**
Institute of Physical Chemistry, Bulgarian Academy of Sciences
Transitions between regimes of new phase growth kinetics; illustration with
growth of equally-sized crystals

10:30–11:00 *Symposium Participants Photo*
Coffee break

Session II **Chairing: Ognyan Petrov**

11:00–11:40 **Ross J. Angel (invited)**
Department of Geosciences, University of Padova, Padova, Italy
In-situ high-pressure X-ray diffraction in materials and mineral science

11:40–12:00 **Milen Gateshki**, Th. Degen, Th. Dortmann
HighScore Plus: crystallography and more

12:00–12:20 H. Sbirikova and **Boris Shivachev**
Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences
Specifics of nucleic acid crystallization for diffraction experiments

12:20–13:40 **Lunch break**

Session III **Chairing: Thomas Kerestedjian**

13:40–14:20 **Ulrich Bismayer (invited)**
Fachbereich Geowissenschaften, Universität Hamburg, Germany
Interfaces in ferroic and non-ferroic systems

14:20–14:40 **Rossitsa Titorenkova***, B. Mihailova, G. Jegova, M. Rashkova
* *Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences*
Raman scattering and IR reflection micro-spectroscopic study of human teeth treated with ER:YAG dental laser

14:40–15:00 **Tzanko Doukov**
representing the SSRL structural biology team
Stanford Synchrotron Radiation Lightsource, SLAC, USA Remote Data Collection at the Stanford Synchrotron Radiation Lightsource

Session IV **Chairing: Boris Shivachev**

15:00–15:40 **Maria Lalia-Kantouri (invited)**, A. Zianna, M. S. Ristic, A. Hatzidimitriou
Laboratory of Inorganic Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, Greece
Cadmium(II) complexes of salicylaldehydes, in the presence or absence of α -diimines

15:40–16:00 **Galina Gencheva**
Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski"
New insights for the design of ruthenium antitumor agents – amino-coordinated Ru(II) and Ru(IV) complexes of 3-amino-2-chloropyridine

16:00–16:20 **Totka Todorova**, Yu. Kalvachev, V. Valtchev & **Lilya Tsvetanova**, S. Ferdov, B. Shivachev, R. Nikolova
Institute of Mineralogy and Crystallography - BAS, Sofia, Bulgaria
Crystal structures of ion exchanged ETS-4 & Synthesis of mordenite type zeolite without organic template

16:20–16:30 **Bas ter Mull** (Industrial Talk)
PANalytical
Empyrean, the comprehensive platform for X-ray diffraction

16:30–16:40 Industrial Talk
Rofa-Rigaku

16:40–19:00 **Welcome party and Poster Session I (odd numbered posters) – Library of UCTM**

19:00–19:30 **Annual meeting of the Bulgarian Crystallographic Society**

Friday 26 September

9:00–9:50 **Chairing: Rositsa Nikolova**
Open public talk (in Bulgarian): **Prof. Georgi Kirov (invited)**
Faculty of Geology and Geography, Sofia University "St. Kl. Ohridski"
Бележки върху развитието на кристалографията в България

Session V **Chairing: Daniela Kovacheva**

9:50–10:30 **Joerg Rothe, (invited)**
Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal (KIT-INE), Karlsruhe, Germany
X-ray absorption fine structure spectroscopy (XAFS) with synchrotron radiation – an introduction

- 10:30–11:00 **Coffee break**
- 11:00–11:40 **Tonya Vitova (invited)**
Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
High energy resolution X-ray absorption spectroscopy and inelastic X-ray scattering investigations of actinide and lanthanide materials
- 11:40–12:00 T. Vitova, S. Mangold, C. Paulmann, V. Marinova, M. Gospodinov,
Boriana Mihailova*
**FB Geowissenschaften, Universität Hamburg, Hamburg, Germany*
Mesoscopic-scale atomic arrangements in Ru-doped perovskite-type relaxor ferroelectrics revealed by X-ray absorption spectroscopy
- 12:00–12:20 **Victor Ivanov**
Faculty of Physics, Sofia University "St. Kl. Ohridski"
Crystallographic structure and vibrational modes of mercury telluride nanowires encapsulated in single walled carbon nanotubes
- 12:20–13:40 **Lunch break**
- Session VI** **Chairing: Galina Gencheva**
- 13:40–14:20 **Biliana Gasharova* (invited)**, Y.-L. Mathis, D. Moss, K. Garbev
** Institute for Photon Science and Synchrotron Radiation / ANKA synchrotron light source, Karlsruhe Institute of Technology, Karlsruhe, Germany*
Synchrotron infrared microspectroscopy: basics and applications in mineralogy and materials science
- 14:20–14:40 **Veronika Karadjova***, M. Wildner, D. Manasieva, D. Stoilova
** Department of Inorganic Chemistry, University of Chemical Technology and Metallurgy, Sofia*
Hydrogen bond strength in some beryllium compounds. Correlation between structural data and infrared spectra
- 14:40–15:20 **Krassimir Garbev* (invited)**, B. Gasharova, P. Stemmermann,
** Institute for Technical Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany*
New insights into the structure of cementitious materials
- 15:20–15:40 **Alexander Karamanov**
Institute of Physical Chemistry, Bulgarian Academy of Sciences
Synthesis, structure and properties of innovative ceramics from industrial wastes
- 15:40–16:00 **Alaa Adam^{1,2}**, E. Lilov, P. Petkov
¹ Physics Department, University of Chemical Technology and Metallurgy, Sofia; ² Physics Department, Faculty of Science, Sohag University, EGYPT
Structural and physicochemical properties of crystalline bismuth chalcogenides
- 16:00–16:10 Industrial Talk
Aquachim
Particle size characterization instruments – innovative solutions from Beckman Coulter
- 16:10–18:30 **Poster Session II (even numbered posters) – Library of UCTM**

Saturday 27 September

Session VII *Chairing: Boriana Mihailova*

9:00–9:40

Emre S. Tasci* (invited), S. Polad , T. Biroł

** Physics Department, Middle East Technical University, Ankara, Turkey*

Hunting for multiferroics via DFT modelling

9:40–10:00

Thomas Kerestedjian

Institute of Geology, Bulgarian Academy of Sciences

Match-2: Single and mixed phase identification from XRD data

10:00–10:20

Diana Nihtianova*, L. Mihaylov, P. Tzvetkov, P. Markov, A. Yordanova, I. Koseva, V. Nikolov

** Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences*

Characterization of nanosized $Al_{2-x}Sc_x(WO_4)_3$ solid solutions by transmission electron microscopy (SAED, HRTEM, XEDS)

10:20–10:50

Coffee break

Session VIII *Chairing: Daniela Karashanova*

10:50–11:30

Rossitza Pentcheva (invited)

Theoretical Physics, Faculty of Physics, University of Duisburg-Essen, Germany

Mechanisms of electronic reconstruction at oxide interfaces: Insights from DFT+U calculations

11:30–11:50

Zara Cherkezova-Zheleva

Institute of Catalysis, Bulgarian Academy of Sciences

Preparation of improved and nanodimensional catalytic materials by mechanochemical method

11:50–12:10

Georgi Avdeev

Institute of Physical Chemistry, Bulgarian Academy of Sciences

Institute of Physical Chemistry, Bulgarian Academy of Sciences

Високотехнологична лаборатория за специализирани рентгенови методи и томография за развитие на еко- и енергоспестяващи технологии и технологии, свързани със здравето

12:30–13:00

Award for the best poster contribution by young scientists

Closing remarks, Rositsa Nikolova, President of BCS

Poster Session

- P_1. M. Abdallah, N. Velikova, Y. Ivanova, Y. Dimitriev – Synthesis and characterization of poly sulfide-functionalized hybrid mesoporous silica
- P_2. B. Angelov, A. Angelova, S. K. Filippov, M. Drechsler, P. Štěpánek, S. Lesieur – Time resolved X-ray scattering of protein loaded lipid nanoparticle
- P_3. V. Angelov, E. Ivanov, R. Kotsilkova – The chemical composition and structure of three phase epoxy/organoclay/gold nanocomposites
- P_4. Z. A. Babakhanova, M. Kh. Aripova, J. Aripov – Studying the structure of quartz-graphite schists using SEM analysis
- P_5. B. Barbov, Yu. Kalvachev – Synthesis of Beta zeolites in the presence of seeds